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Lecture Notes

The Pancharatnam-Berry Phase

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¹This Section closely follows Ref.[10]

Chapter 1

Introduction

In 1984 Berry [1] addressed the case of a quantum system undergoing a unitary, cyclic evolution under the action of a time-dependent Hamiltonian. The evolution was supposed to be adiabatic, i.e., the time scale at which the quantum system evolved was supposed to be much shorter than the time scale of the changing Hamiltonian. Until Berry's study it was assumed that, after a cycle, the quantum state would acquire a so-called dynamical phase, with no physical meaning. Such a phase could be eliminated by redefining the quantum state through a "gauge" transformation of the form $|\psi\rangle \rightarrow e^{i\alpha} |\psi\rangle$. However, Berry discovered that there was a phase, additional to the dynamical phase, that could not be "gauged away" and whose origin was "geometric" or topological, i.e., it depended on the path that $|\psi\rangle$ traced out in the parameter space defined by those parameters to which the Hamiltonian owed its time dependence. Berry's discovery was the starting point for a great amount of investigations that brought to light topological aspects of both quantum and classical systems. Berry's phase was soon recognized as a special case of more general phases that showed up when dealing with topological aspects of different systems. For example, the Aharonov-Bohm phase could be understood as a geometric phase. The rotation angle acquired by a parallel-transported vector after completing a closed loop in a space-time region deformed by the presence of a gravitational field is also a geometric, Berry-like phase. The same holds true for the precession of the plane of oscillation of a pendulum, due to the Earth rotation (a Foucault pendulum).

Berry's original formulation was directly applicable to the case of a spin-1/2 system evolving under the action of a slowly varying magnetic field that undergoes cyclic changes. Now, a spin-1/2 system is a special case of a two-level system. Another instances are two-level atoms and polarized light. Also here we can expect to find geometric phases. In fact, the first experimental test of Berry's phase was done using polarized, classical light [2]. Pancharatnam [3] anticipated Berry's phase when he proposed, in 1956, how to decide whether two polarization states are, or are not, "in phase". Pancharatnam's prescription is an operational one, based upon observing whether the intensity of the interferogram formed by two polarized beams has maximal intensity. In that case, the two polarized beams are said to be "in phase". Such a definition is analogous to the definition of distant parallelism in differential geometry. Polarized states can be subjected to different transformations which could be cyclic or not, adiabatic or not, unitary or not. And in all cases Pancharatnam's definition applies. Pancharatnam's phase bore therefore an anticipation and – at the same time – a generalization of Berry's phase. Indeed, Berry's assumptions that the evolution was cyclic, adiabatic and unitary, showed up to be unnecessary conditions for a geometric phase to appear. This was made clear through the contributions of several authors that addressed the issue right after Berry published his seminal results [4, 5].

Pancharatnam's approach, general as it was when viewed as pregnant of so many concepts

related to geometric phases, underlay however two important restrictions. It addressed non-orthogonal and at the same time pure, viz totally, polarized states. Here again the assumed restrictions turned out to be unnecessary. Indeed, it was recently proposed how to decide whether two orthogonal states are in phase or not [6]. Mixed states have also been addressed [7] in relation to geometric phases which – under appropriate conditions – can be exhibited as well-defined objects underlying the evolution of such states.

The present Lectures should provide an overview of the Pancharatnam-Berry phase by introducing it first within Berry's original approach and then through the kinematic approach [8] that was advanced by Simon and Mukunda some years after Berry's discovery. The kinematic approach brings to the fore the most essential aspects of geometric phases, something that was not yet accomplished when Berry first addressed the issue. As has often been the case in physics, a fundamental discovery that is made by addressing a particular issue, can show afterwards to bear a rather unexpected generality and applicability. Berry's discovery ranks among this kind of fundamental advances.

Chapter 2

The adiabatic and cyclic case

2.1 A general approach

Let us consider a time-dependent Hamiltonian $H(t)$ and a state $|\psi(t)\rangle$ evolving under its action:

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = H(t) |\psi\rangle. \quad (2.1)$$

The eigenvalue equation for $H(t)$ can be solved for each t :

$$H(t) |a(t)\rangle = E(t) |a(t)\rangle, \quad (2.2)$$

whereby we assume that the eigenvalues $E(t)$ are non-degenerate. The phase of $|a(t)\rangle$ can be freely chosen. Let us choose it so, that

$$\langle a(t) | \dot{a}(t) \rangle = 0. \quad (2.3)$$

Then, under the assumption of adiabatic evolution and the system starting in the eigenstate $|a(0)\rangle$, it can be shown that an approximate solution of Eq.(2.1) is given by

$$|\psi(t)\rangle \approx \exp\left(-\frac{i}{\hbar} \int_0^t E(s) ds\right) |a(t)\rangle. \quad (2.4)$$

This result was obtained by Fock in 1928 [9], and for half a century it was taken for granted that by a phase choice Eq.(2.4) would give an adiabatic solution. However, Fock did not consider cyclic Hamiltonians. For a cyclic Hamiltonian whose period is T , we have that $H(T) = H(0)$. The question addressed by Berry was whether $|\psi(T)\rangle = |\psi(0)\rangle = |a(0)\rangle$, up to the “dynamical” phase-factor $\exp\left(-i \int_0^T E(s) ds / \hbar\right)$. What Berry found was that $|\psi(T)\rangle = \exp(-i\Phi_{tot}/\hbar) |\psi(0)\rangle$; but that the total, accumulated phase Φ_{tot} was not, in general, the dynamical phase. Indeed, Berry found that Φ_{tot} contained besides the dynamical, a geometric part:

$$\Phi_{tot} = \Phi_g + \Phi_{dyn}. \quad (2.5)$$

That is, besides the expected dynamical part

$$\Phi_{dyn} = \int_0^T E(s) ds = \int_0^T \langle a(s) | H(s) | a(s) \rangle ds, \quad (2.6)$$

there was an additional contribution Φ_g whose geometrical origin we will elucidate in what follows.

Let us take the following *ansatz* as a solution for Eq.(2.1):

$$|\psi(t)\rangle \approx \exp\left(\frac{i}{\hbar}\gamma(t) - \frac{i}{\hbar}\int_0^t E(s)ds\right) |a(t)\rangle, \quad (2.7)$$

with $\gamma(0) = 0$, so that initially $|\psi(0)\rangle = |a(0)\rangle$. Then,

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = (-\dot{\gamma}(t) + E(t)) |\psi\rangle + i\hbar \exp\left(\frac{i}{\hbar}\gamma(t) - \frac{i}{\hbar}\int_0^t E(s)ds\right) |\dot{a}(t)\rangle \quad (2.8)$$

$$= H(t) |\psi\rangle + \exp\left(\frac{i}{\hbar}\gamma(t) - \frac{i}{\hbar}\int_0^t E(s)ds\right) [-\dot{\gamma}(t)|a(t)\rangle + i\hbar|\dot{a}(t)\rangle] \quad (2.9)$$

For Eq.(2.1) to be satisfied, we can take

$$\dot{\gamma}(t) \approx i\hbar \langle a(t) | \dot{a}(t) \rangle, \quad (2.10)$$

$$\gamma(t) \approx i\hbar \int_0^t \langle a(s) | \dot{a}(s) \rangle ds. \quad (2.11)$$

Now, because $H(T) = H(0)$, and because we have assumed non-degenerate eigenvalues ($E(T) = E(0)$), the eigenstates $|a(T)\rangle$ and $|a(0)\rangle$ can differ from one another only through a phase-factor that can be set to one: $|a(T)\rangle = |a(0)\rangle$. We have thus, because of Eq.(2.7) and $|a(T)\rangle = |a(0)\rangle = |\psi(0)\rangle$, that

$$|\psi(T)\rangle \approx \exp\left(\frac{i}{\hbar}\gamma(T) - \frac{i}{\hbar}\int_0^T E(s)ds\right) |\psi(0)\rangle. \quad (2.12)$$

Note that Eq.(2.7) cannot hold exactly, but only as an approximation. This is because the condition we have imposed on $\gamma(t)$, Eq.(2.11), requires that $|a(t)\rangle$ satisfies the equation

$$|\dot{a}(t)\rangle = \langle a(t) | \dot{a}(t) \rangle |a(t)\rangle, \quad (2.13)$$

for the second term in Eq.(2.9) to be zero. Such a condition is generally not satisfied.

In order to see that $\gamma(t)$ has a geometrical origin we need to make our treatment more specific. By so doing, we will also introduce some concepts that will be useful for several purposes.

2.2 ¹Berry's approach

2.2.1 Berry's phase

The time-dependence of $H(t)$ means that the system under consideration is non-conservative. This happens when the system is part of a larger system, i.e., when it evolves under the influence of an environment. The configuration of the environment can generally be specified by a set of parameters (R_1, R_2, \dots) . For a changing environment the R_i are time-dependent, and so also the observables of the system, one of which is the Hamiltonian: $H(R(t)) \equiv H(R_1(t), R_2(t), \dots) = H(t)$. The evolution of the quantum system is ruled by the Schrödinger equation, Eq.(2.1), or more generally, by the Liouville-von Neumann equation

¹This Section closely follows Ref.[10]

$$i\hbar \frac{d\rho(t)}{dt} = [H(R(t)), \rho(t)] \quad (2.14)$$

for the density operator ρ . For a pure state $\rho(t) = |\psi(t)\rangle \langle \psi(t)|$. An environmental process is given through $t \rightarrow R(t)$, that is, through the curve that the parameters R describe in the parameter space. To such a process it corresponds a curve described by the state vector $|\psi(t)\rangle$ in the Hilbert space \mathcal{H} to which it belongs, as well as a corresponding curve described by $\rho(t) = |\psi(t)\rangle \langle \psi(t)|$ in the “projection space” $\mathcal{P}(\mathcal{H})$ to which ρ belongs. We will assume that for any R , there is an orthonormal basis $|n; R\rangle$ such that

$$H(R) |n; R\rangle = E_n(R) |n; R\rangle. \quad (2.15)$$

An environmental process $R(t)$ is called periodic with period T , whenever $R(T) = R(0)$, $E_n(R(T)) = E_n(R(0))$, and $|n; R(T)\rangle \langle n; R(T)| = |n; R(0)\rangle \langle n; R(0)|$. In general, however, the $|n; R\rangle$ need not be single-valued:

$$|n; R(T)\rangle = e^{i\alpha_n} |n; R(0)\rangle, \quad (2.16)$$

in general. Of course, we can change the eigenbasis according to $|n; R\rangle \rightarrow |n; R'\rangle = e^{i\alpha_n(R)} |n; R\rangle$. This is called a gauge transformation.

The adiabatic approximations consists in taking as an approximate solution of Eq.(2.14) the following one:

$$\rho(t) = |\psi(t)\rangle \langle \psi(t)| \approx |n; R(t)\rangle \langle n; R(t)|. \quad (2.17)$$

When $R(t)$ traces back a closed path ($R(T) = R(0)$) so also does $\rho(t)$ under the adiabatic approximation: $|\psi(T)\rangle \langle \psi(T)| \approx |n; R(T)\rangle \langle n; R(T)| = |n; R(0)\rangle \langle n; R(0)|$. However, the state $|\psi(t)\rangle$ itself may acquire a phase. That $|\psi(t)\rangle \langle \psi(t)| \approx |n; R(t)\rangle \langle n; R(t)|$ can only be an approximation follows from observing that $[H(R(t)), |n; R(t)\rangle \langle n; R(t)|] = 0$, so that only stationary states $|\psi(t)\rangle \langle \psi(t)| = |n; R(t)\rangle \langle n; R(t)|$ could be solutions of Eq.(2.14). In general, the adiabatic assumption is incompatible with the requirement imposed by Eq.(2.14) for the evolution of the physical states. Let us see under which conditions holds the adiabatic approximation. In general, we can write $|\psi(t)\rangle = \sum_k c_k(t) |k; R(t)\rangle$. If $|\psi(0)\rangle = |n; R(0)\rangle$, the adiabatic approximation means that $|\psi(t)\rangle \approx c_n(t) |n; R(t)\rangle$, with $c_n(0) = 1$. By replacing such a $|\psi(t)\rangle$ in the Schrödinger equation one easily obtains the necessary and sufficient condition for the adiabatic assumption to hold true:

$$\langle k; R(t) | \frac{d}{dt} |n; R(t)\rangle \approx 0, \quad \text{for all } k \neq n. \quad (2.18)$$

By using Eq.(2.15) this condition can be written as

$$\frac{\langle k; R(t) | dH(t)/dt |n; R(t)\rangle}{E_n(R) - E_k(R)} \approx 0, \quad \text{for all } k \neq n. \quad (2.19)$$

Hence, the transition frequencies of the evolving system, $(E_n(R) - E_k(R))/\hbar$, set the time scale for the variation of $H(t)$ to be considered as “adiabatic”.

Now, the coefficient $c_n(t)$ in the adiabatic approximation $|\psi(t)\rangle \approx c_n(t) |n; R(t)\rangle$ must satisfy the equation

$$\frac{dc_n}{dt} = -c_n \left[iE_n(t) + \langle n; R(t) | \frac{d}{dt} |n; R(t)\rangle \right], \quad (2.20)$$

whose solution is

$$c_n(t) = \exp \left[-i \int_0^t E_n(s) ds \right] \exp \left[- \int_0^t \langle k; R(s) | \frac{d}{ds} | n; R(s) \rangle ds \right] \equiv \exp(-i\Phi_{dyn}(t)) \exp(i\gamma_n(t)). \quad (2.21)$$

Hence,

$$|\psi(t)\rangle \approx c_n(t) |n; R(t)\rangle = \exp(i\Phi_{dyn}(t)) \exp(i\gamma_n(t)) |n; R(t)\rangle. \quad (2.22)$$

The geometric phase γ_n can also be written as

$$\gamma_n(t) = i \int_0^t \langle n; R(s) | \frac{d}{ds} | n; R(s) \rangle ds \quad (2.23)$$

$$= i \int_{R(0)}^{R(t)} \langle n; R | \frac{\partial}{\partial R_k} | n; R \rangle dR_k \equiv \int_{R(0)}^{R(t)} \mathbf{A}^{(n)} \cdot d\mathbf{R}, \quad (2.24)$$

with the vector potential $\mathbf{A}^{(n)} = i \langle n; R | \nabla | n; R \rangle$, which is named the *Mead-Berry vector potential*. Eq.(2.24) makes it clear that γ_n depends on the path defining the environmental process, viz., the path connecting the points $R(0)$ and $R(t)$ in parameter space. This gives us a clue as to the geometrical nature of γ_n . Now, one can straightforwardly prove that under a gauge transformation $|n; R\rangle \longrightarrow |n; R\rangle' = e^{i\alpha_n(R)} |n; R\rangle$ the vector potential transforms as

$$\mathbf{A}^{(n)} \longrightarrow \mathbf{A}'^{(n)} = \mathbf{A}^{(n)} - \nabla \alpha_n(R). \quad (2.25)$$

As a consequence then,

$$\gamma_n(t) \longrightarrow \gamma_n'(t) = \gamma_n(t) - [\alpha_n(R(t)) - \alpha_n(R(0))] \quad (2.26)$$

and we can use this gauge freedom to remove the phase factor $\exp(i\gamma_n)$ in Eq.(2.22). Indeed, we can repeat the calculations leading to Eq.(2.22) but using $|n; R\rangle' = e^{i\alpha_n(R)} |n; R\rangle$ instead of $|n; R\rangle$. We thus obtain an equation like Eq.(2.22) but with primed quantities. We can then choose $\alpha_n(R(t)) = -\gamma_n'(t)$ (modulo 2π) and so obtain

$$|\psi(t)\rangle \approx \exp(i\Phi_{dyn}(t)) |n; R(t)\rangle. \quad (2.27)$$

This is what Fock made, exploiting the freedom one has to choose $\alpha_n(R(t))$. However, when we have a closed path C we cannot do this anymore. This is because $R(T) = R(0)$ and $\exp(i\alpha_n(T)) = \exp(i\alpha_n(0))$, so that $\alpha_n(T) = \alpha_n(0)$ modulo 2π . Hence, because of Eq.(2.26),

$$\gamma_n(T) \longrightarrow \gamma_n'(T) = \gamma_n(T) - 2\pi m, \quad (2.28)$$

with m an integer. We conclude that $\gamma_n(T)$ is invariant, modulo 2π , under gauge transformations, and we have finally,

$$|\psi(T)\rangle = \exp(-i\Phi_{dyn}(T)) \exp(i\gamma_n(T)) |\psi(0)\rangle, \quad (2.29)$$

with

$$\Phi_{dyn}(T) = \int_0^T E_n(t) dt, \quad (2.30)$$

$$\gamma_n(T) = \oint_C \mathbf{A}^{(n)} \cdot d\mathbf{R}. \quad (2.31)$$

The vector potential $\mathbf{A}^{(n)}$ behaves very much like an electromagnetic potential. The phase factors $\exp(i\alpha_n(R))$ form the group $U(1)$, hence the name “gauge transformations” given to the transformations $|n; R\rangle \rightarrow |n; R\rangle' = e^{i\alpha_n(R)} |n; R\rangle$. As in electromagnetism, we can also here introduce a field tensor $\mathbf{F}^{(n)}$ whose components are

$$F_{ij}^{(n)} = \frac{\partial}{\partial R_i} A_j^{(n)} - \frac{\partial}{\partial R_j} A_i^{(n)}. \quad (2.32)$$

Geometrically, $\mathbf{F}^{(n)}$ has the meaning of a “curvature”. In differential geometry, where the language of differential forms is used, to $\mathbf{A}^{(n)}$ it corresponds a one-form, while to $\mathbf{F}^{(n)}$ it correspond a two-form.

When the parameter space is three-dimensional, Eq.(2.32) can be written as

$$\mathbf{F}^{(n)} = \nabla \times \mathbf{A}^{(n)}. \quad (2.33)$$

Eq.(2.31) can then be written as

$$\gamma_n(T) = \int_S \mathbf{F}^{(n)} \cdot d\mathbf{S}, \quad (2.34)$$

with the surface element $d\mathbf{S}$ directed normally to the surface S whose boundary is the curve C .

As we have seen, Berry's phase $\gamma_n(T)$ has been introduced by considering unitary, cyclic and adiabatic evolutions. This was Berry's original approach. Soon afterwards his approach was generalized by Aharonov and Anandan [4] to the non-adiabatic case, and by Samuel and Bhandari [5] to the noncyclic case. Unitarity was also shown to be non-essential by addressing the issue from a purely kinematic point of view. This was done by Mukunda and Simon [8], whose approach we present in the next Section. Before that, it will be useful to discuss in more detail some topological aspects of Berry's phase. They will illustrate how deep can go the notion of a geometric phase.

2.2.2 Angular momentum and monopoles

A paradigmatic case in which Berry's phase has been amply studied is that of a quantum spin-1/2 particle subjected to the action of a rotating magnetic field. We can write such a field as $\mathbf{B}(t) = B\mathbf{n}(t)$, with a rotating unit vector $\mathbf{n}(t)$. The parameter space of this system is thus S^2 , the unit sphere in \mathbb{R}^3 . The Hamiltonian of this system is

$$H(R(t)) = -B \frac{ge}{2mc} \mathbf{n}(t) \cdot \mathbf{S}, \quad (2.35)$$

where e is the electron's charge, g the Landé factor, and $\mathbf{S} = \hbar \vec{\sigma}/2$, with $\vec{\sigma}$ representing a vector of Pauli matrices. For particles of arbitrary spin the above Hamiltonian reads

$$H(\mathbf{n}(t)) = -B \frac{ge}{2mc} \mathbf{n}(t) \cdot \mathbf{J} \equiv b\mathbf{n}(t) \cdot \mathbf{J}. \quad (2.36)$$

When $\mathbf{B}(t)$ rotates uniformly with angular velocity ω around the z -axis its component B_3 remains constant. Let us write $\mathbf{B}(t) = B(\cos \omega t \sin \theta, \sin \omega t \sin \theta, \cos \theta)$. The eigenvectors of the corresponding Hamiltonian can be shown to satisfy

$$H(\mathbf{n}(t))|k; \mathbf{n}(t)\rangle = b\mathbf{n}(t) \cdot \mathbf{J}|k; \mathbf{n}(t)\rangle = bk|k; \mathbf{n}(t)\rangle, \quad (2.37)$$

with

$$J_3|k; \mathbf{n}(0)\rangle = k|k; \mathbf{n}(0)\rangle. \quad (2.38)$$

This immediately follows from noting that $H(\mathbf{n}(t))$ and J_3 are related to one another by a unitary transformation: $H(\mathbf{n}(t)) = bU(\theta, \omega t)J_3U^{-1}(\theta, \omega t)$, with $U(\theta, \omega t) = \exp(-i\omega t J_3) \exp(-i\theta J_2)$. We note that the eigenvalues of $H(R)$ are constant ($E(R(t)) = bk$), although its eigenvectors are not: $|k; \mathbf{n}(t)\rangle = U(\theta, \omega t)|k; \mathbf{n}(0)\rangle$.

If the system has spherical symmetry, and hence $H(R)$ commutes with \mathbf{J}^2 , then the $|k; R\rangle$ are also eigenvectors of \mathbf{J}^2 for eigenvalues that can be denoted as $j(j+1)$. In such a case, the values of k are given by $k = -j, -j+1, \dots, j-1, j$ and it can be shown that j must be an integer or a half-integer, so that $k = 0, \pm 1/2, \pm 1, \pm 3/2, \dots$. But there are cases in which $H(R)$ does not commute with \mathbf{J}^2 , as it occurs, e.g., when the system has only axial symmetry (a diatomic molecule would be an important example of this case). Nevertheless, also in such a situation one can derive from considerations based on Berry's phase that $k = 0, \pm 1/2, \pm 1, \pm 3/2, \dots$, as we shall see. This nicely illustrates how Berry's approach can bring out rather unexpectedly the topological root of some known results. In the present case these topological properties are also connected with Dirac's monopoles.

The topology we are referring to in the present case is the topology of the unit sphere S^2 . As well known, it is not possible to assign coordinates to all points of S^2 by a single patch. We need at least two of them. To be concrete, let us use spherical coordinates to parametrize the points of S^2 : then, all of S^2 , with exception of two points, is univocally given by $\mathbf{n}(\theta, \varphi) = (\cos \varphi \sin \theta, \sin \varphi \sin \theta, \cos \theta)$, with $0 \leq \theta \leq \pi$ and $0 \leq \varphi < 2\pi$. The exceptional points are the north pole $\mathbf{e}_3 = (0, 0, 1)$ and the south pole $-\mathbf{e}_3$, for which the value of φ is arbitrary.

Let us see the consequences that the topology of S^2 has for Berry's phase. To this end, let us consider the following Hamiltonian, a particular case of which was the Hamiltonian of Eq.(2.36). Let us define $H(\mathbf{n}(\theta, \varphi)) = b\mathbf{n}(\theta, \varphi) \cdot \mathbf{J}$. Its eigenvectors can be obtained from those of J_3 by a unitary transformation. Indeed, let us write $J_3|k; \mathbf{e}_3\rangle = k|k; \mathbf{e}_3\rangle$ and denote by $|k; \mathbf{n}(\theta, \varphi)\rangle$ the eigenvectors of $\mathbf{n}(\theta, \varphi) \cdot \mathbf{J}$. Last ones can be obtained from the $|k; \mathbf{e}_3\rangle$ by applying to them a rotation that brings \mathbf{e}_3 to $\mathbf{n}(\theta, \varphi)$: $\mathcal{R}(\theta, \varphi)\mathbf{e}_3 = \mathbf{n}(\theta, \varphi)$. A convenient choice for $\mathcal{R}(\theta, \varphi)$ is given by

$$\mathcal{R}(\theta, \varphi) = \mathcal{R}_3(\varphi)\mathcal{R}_2(\theta)\mathcal{R}_3(-\varphi). \quad (2.39)$$

$\mathcal{R}_3(\varphi)\mathcal{R}_2(\theta)$ would also bring \mathbf{e}_3 to $\mathbf{n}(\theta, \varphi)$; but the last factor $\mathcal{R}_3(-\varphi)$ in Eq.(2.39) serves to make $\mathcal{R}(0, \varphi) = I$. The unitary transformation corresponding to $\mathcal{R}(\theta, \varphi)$ is

$$U_N(\theta, \varphi) = \exp(-i\varphi J_3) \exp(-i\theta J_2) \exp(i\varphi J_3). \quad (2.40)$$

Thus,

$$|k; \mathbf{n}(\theta, \varphi)\rangle_N \equiv |k; \theta, \varphi\rangle_N = U_N(\theta, \varphi)|k; \mathbf{e}_3\rangle. \quad (2.41)$$

Our choice of $U_N(\theta, \varphi)$ smoothly assigns to each $\mathbf{n}(\theta, \varphi)$ a unique eigenvector $|k; \theta, \varphi\rangle$, with the exception of the south pole (hence the label N), for which $\theta = \pi$. In such a case, using that $\exp(-i\pi J_2) \exp(i\varphi J_3) = \exp(-i\varphi J_3) \exp(-i\pi J_2)$, Eq.(2.41) gives

$$\begin{aligned} |k; \pi, \varphi\rangle_N &= \exp(-i\varphi J_3) \exp(-i\pi J_2) \exp(i\varphi J_3) |k; \mathbf{e}_3\rangle = \exp(-i\pi J_2) \exp(2i\varphi J_3) |k; \mathbf{e}_3\rangle \\ &= \exp(-i\pi J_2) e^{2ik\varphi} |k; \mathbf{e}_3\rangle \end{aligned} \quad (2.42)$$

Thus, for the different values of φ in the interval $0 \leq \varphi < 2\pi$ we obtain different state vectors $|k; \pi, \varphi\rangle$, so that we have no single-valued assignment at the south pole for this parametrization

of S^2 . At the north pole the assignment is single-valued, because $\mathcal{R}(0, \varphi) = I$, as we have seen. We thus have $|k; 0, \varphi\rangle = |k; 0, 0\rangle = |k; \mathbf{e}_3\rangle$.

A parametrization that is single-valued at the south pole can be obtained by gauge transforming the $|k; \theta, \varphi\rangle$ according to

$$|k; \theta, \varphi\rangle_S = e^{-i2k\varphi} |k; \theta, \varphi\rangle_N = \exp(-i\varphi J_3) \exp(-i\theta J_2) \exp(-i\varphi J_3) |k; \mathbf{e}_3\rangle \equiv U_S(\theta, \varphi) |k; \mathbf{e}_3\rangle. \quad (2.43)$$

At the south pole we obtain, similarly to what we did before, that $|k; \pi, \varphi\rangle_S = e^{-i\pi J_2} |k; \mathbf{e}_3\rangle$, so that we have now a single-value assignment at this point. However, at the north pole we have now the multiple-valued assignment $|k; 0, \varphi\rangle_N = e^{-i2\pi\varphi} |k; \mathbf{e}_3\rangle$. In order to have a single-valued assignment in all of S^2 we need at least two patches: $O_N = S^2 - \{-\mathbf{e}_3\}$ and $O_S = S^2 - \{\mathbf{e}_3\}$. In the overlap $O_N \cap O_S$ either parametrization can be used. Corresponding to these two parametrizations we have two vector potentials: $\mathbf{A}_m^{(k)} = i_m \langle k; R | \nabla_R | k; R \rangle_m$, $m = N, S$. For O_N the eigenvectors are given by $|k; \theta, \varphi\rangle_N = U_N(\theta, \varphi) |k; \mathbf{e}_3\rangle$, while for O_S they are $|k; \theta, \varphi\rangle_S = U_S(\theta, \varphi) |k; \mathbf{e}_3\rangle$. We can then calculate $\mathbf{A}_m^{(k)}$ as

$$\mathbf{A}_m^{(k)} = i \langle k; \mathbf{e}_3 | U_m^\dagger \left(\mathbf{e}_r \frac{\partial}{\partial r} + \mathbf{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \mathbf{e}_\varphi \frac{1}{\sin \theta} \frac{\partial}{\partial \varphi} \right) U_m | k; \mathbf{e}_3 \rangle. \quad (2.44)$$

We obtain

$$\mathbf{A}_{O_N}^{(k)} = \frac{k(\cos \theta - 1)}{r \sin \theta} \mathbf{e}_\varphi, \quad \theta \neq \pi, \quad (2.45)$$

$$\mathbf{A}_{O_S}^{(k)} = \frac{k(\cos \theta + 1)}{r \sin \theta} \mathbf{e}_\varphi, \quad \theta \neq 0. \quad (2.46)$$

We see that $\mathbf{A}_{O_N}^{(k)}$ and $\mathbf{A}_{O_S}^{(k)}$ are related to each other by a gauge transformation:

$$\mathbf{A}_{O_S}^{(k)} = \mathbf{A}_{O_N}^{(k)} + \frac{2k}{r \sin \theta} \mathbf{e}_\varphi = \mathbf{A}_{O_N}^{(k)} - \nabla \alpha, \quad \text{with } \alpha = -2k\varphi. \quad (2.47)$$

The corresponding field tensor $\mathbf{F}^{(k)} = \nabla \times \mathbf{A}^{(k)}$ is given by

$$\mathbf{F}^{(k)} = -\frac{k}{r^2} \mathbf{e}_r. \quad (2.48)$$

We recognize here the field produced by a monopole located at the origin of our coordinate system. In terms of this field we can now calculate the geometric phase corresponding to a closed curve C . It is given by

$$\gamma_k(C) = \int_S \mathbf{F}^{(k)} \cdot d\mathbf{S} = \int_S F_r^k r^2 \sin \theta d\theta d\varphi = -k \int_S \sin \theta d\theta d\varphi = -k \int_S d\Omega, \quad (2.49)$$

with S being any surface whose boundary $\partial S = C$, and $d\Omega$ the element of solid angle, or area element of the unit sphere. We have thus the important result

$$\gamma_k(C) = -k\Omega(C). \quad (2.50)$$

$\gamma_k(C)$ is gauge-independent, as $\mathbf{F}^{(k)}$ is. Our calculation is therefore independent of what surface S we choose. For example, S could be contained in O_N , in which case its normal points out of the sphere S^2 . If instead $S \subset O_S$, its normal points into the sphere S^2 . Let us denote the first surface by S_N and the second one by S_S . They have as common boundary C and their

union is the whole sphere S^2 . Hence, because of the opposite pointing directions of the normals to S_N and to S_S , we have

$$\gamma_k(C) = k \int_{S_N} d\Omega = -k\Omega(C) = k \left(\int_{S^2} d\Omega - \int_{S_S} d\Omega \right) = k(4\pi - \Omega(C)) + 2\pi n, \quad n = \pm 0, \pm 1, \pm 2, \dots, \quad (2.51)$$

where we have included the term $2\pi n$ to take into account that $\gamma_k(C)$ is defined only modulo 2π . From Eq.(2.51) we see that $-k\Omega(C) = 4\pi k - k\Omega(C) + 2n\pi$, $n = \pm 0, \pm 1, \pm 2, \dots$, and so we arrive at the conclusion that $k = 0, \pm 1/2, \pm 1, \pm 3/2, \dots$ *without* having assumed spherical symmetry: \mathbf{J}^2 may not commute with $H(R)$. This illustrates how some results can have in fact topological roots. In the present case, it is the topology of S^2 that shows up as a common root to the geometric phase and to monopoles. In both cases the topology of the parameter space shows its non-trivial structure. In the case of the monopole we can say that it represents a singularity which makes a space region multiple-connected. In the case of the sphere, its topology precludes a covering by a single patch. In both cases, the corresponding vector potentials \mathbf{A} are non-integrable. There is no single-valued function $\alpha(R)$ for which $\mathbf{A} = \nabla\alpha$.

Chapter 3

The kinematic approach

3.1 Total, geometric, and dynamical phases

We will see now how all of the essential features we have seen before emerge from a purely kinematic approach. Let us start by defining \mathcal{H}_0 as the subset of the Hilbert space \mathcal{H} whose elements are normalized nonzero vectors $|\psi\rangle$. A curve \mathcal{C}_0 in \mathcal{H}_0 is defined through vectors $|\psi(s)\rangle$ that are continuous functions of some parameter $s \in [s_1, s_2]$. Because $|\psi(s)\rangle$ is normalized, $\langle\psi(s)|\dot{\psi}(s)\rangle + \langle\dot{\psi}(s)|\psi(s)\rangle = 0$, which means that $Re\langle\psi(s)|\dot{\psi}(s)\rangle = 0$, so that

$$\langle\psi(s)|\dot{\psi}(s)\rangle = iIm\langle\psi(s)|\dot{\psi}(s)\rangle. \quad (3.1)$$

Under the gauge transformation $|\psi(s)\rangle \rightarrow |\psi'(s)\rangle = \exp(i\alpha(s))|\psi(s)\rangle$ the curve $\mathcal{C}_0 \rightarrow \mathcal{C}'_0$ and $Im\langle\psi(s)|\dot{\psi}(s)\rangle \rightarrow Im\langle\psi'(s)|\dot{\psi}'(s)\rangle = Im\langle\psi(s)|\dot{\psi}(s)\rangle + \dot{\alpha}(s)$. This suggests that we define the following gauge-invariant quantity, as a functional of the curve \mathcal{C}_0 , and hence of \mathcal{C}'_0 :

$$\Phi_g(\mathcal{C}_0) = \arg\langle\psi(s_1)|\psi(s_2)\rangle - Im \int_{s_1}^{s_2} \langle\psi(s)|\dot{\psi}(s)\rangle ds. \quad (3.2)$$

For such a quantity holds true not only that it is gauge invariant, i.e., $\Phi_g(\mathcal{C}_0) = \Phi_g(\mathcal{C}'_0)$, but it is also invariant under changes of the parameter s . That is, Φ_g remains the same if we replace s by another parameter s' which is a monotonically increasing function of s . Gauge and reparametrization invariance mean that in spite of having defined Φ_g in terms of $|\psi(s)\rangle$ and the curve \mathcal{C}_0 , it is in fact a quantity that depends on some equivalent classes of $|\psi(s)\rangle$ and \mathcal{C}_0 . Indeed, the set $\{|\psi'\rangle = \exp(i\alpha)|\psi\rangle\}$ whose representative element is $|\psi\rangle$, constitutes an equivalence class. The space spanned by such equivalence classes is called the “ray space” \mathcal{R}_0 . Instead of working with equivalence classes we can work with projectors: $|\psi\rangle\langle\psi|$, whereby each projector corresponds to an equivalence class. That is, the whole set of vectors $\{|\psi'\rangle = \exp(i\alpha)|\psi\rangle\}$ projects onto the object $|\psi\rangle\langle\psi|$ by means of a projection map $\pi : \mathcal{H}_0 \rightarrow \mathcal{R}_0$. In particular, the curves $\mathcal{C}_0, \mathcal{C}'_0$ which are connected to one another by a gauge transformation, constitute also an equivalence class. Under π , they project onto a curve $C_0 \subset \mathcal{R}_0$. What we have seen above is that Φ_g is in fact a functional not of \mathcal{C}_0 , or \mathcal{C}'_0 , but of C_0 , which can be seen as the curve defined by $|\psi(s)\rangle\langle\psi(s)|$. We call then Φ_g the “geometric phase” associated with the curve $C_0 \subset \mathcal{R}_0$. We should then better write $\Phi_g(C_0)$, though the actual calculation of such a quantity requires that we choose

what is called a “lift” of C_0 ; that is, any curve \mathcal{C}_0 in the equivalence class that projects onto C_0 : $\pi(\mathcal{C}_0) = C_0$.

$\Phi_g(C_0)$ has been defined as a sum of two terms in Eq.(3.2). Each of these terms deserves a separate definition:

$$\Phi_{tot}(\mathcal{C}_0) = \arg\langle\psi(s_1)|\psi(s_2)\rangle, \quad (3.3)$$

$$\Phi_{dyn}(\mathcal{C}_0) = \text{Im} \int_{s_1}^{s_2} \langle\psi(s)|\dot{\psi}(s)\rangle ds. \quad (3.4)$$

$\Phi_{tot}(\mathcal{C}_0)$ is the *total phase* of \mathcal{C}_0 , also known as the Pancharatnam phase. It is thus defined as the argument of the complex number $\langle\psi(s_1)|\psi(s_2)\rangle = |\langle\psi(s_1)|\psi(s_2)\rangle| e^{i\alpha}$. Later on, we will discuss the physical meaning of this phase in the context of polarized states, the case addressed by Pancharatnam. $\Phi_{dyn}(\mathcal{C}_0)$ is the *dynamical phase* of \mathcal{C}_0 . We see thus that even though both $\Phi_{tot}(\mathcal{C}_0)$ and $\Phi_{dyn}(\mathcal{C}_0)$ are functionals of \mathcal{C}_0 their difference, Φ_g , is a functional of C_0 :

$$\Phi_g(C_0) = \Phi_{tot}(\mathcal{C}_0) - \Phi_{dyn}(\mathcal{C}_0). \quad (3.5)$$

Let us stress that the present definition of the geometric phase does not rest on the assumptions originally made by Berry. $\Phi_g(C_0)$ has been introduced in terms of an evolution of state vectors $|\psi(s)\rangle$ that does not need to be unitary nor adiabatic. Furthermore, the path \mathcal{C}_0 does not need to be closed and, hence, no cyclic property needs to be invoked. Now, for a given C_0 in ray space, we can choose different lifts in order to calculate $\Phi_g(C_0)$. We can exploit this freedom to express $\Phi_g(C_0)$ as it is most convenient to our tasks. For example, we can always make $\Phi_{tot}(\mathcal{C}_0) = 0$, by properly choosing the phase of, say, $|\psi(s_2)\rangle$. In that case, $\Phi_g(C_0) = -\Phi_{dyn}(\mathcal{C}_0)$. On the other hand, we can also make $\Phi_{dyn}(\mathcal{C}_0) = 0$ by choosing what is called a “*horizontal lift*”. This is a lift for which $\text{Im}\langle\psi(s)|\dot{\psi}(s)\rangle = 0$. Because, as we saw, $\text{Re}\langle\psi(s)|\dot{\psi}(s)\rangle = 0$, for a horizontal lift it holds that $\langle\psi(s)|\dot{\psi}(s)\rangle = 0$ and $\Phi_g(C_0) = \Phi_{tot}(\mathcal{C}_0)$. In order to obtain a horizontal lift we need only submit, if necessary, an arbitrarily chosen lift, that is defined by $|\psi(s)\rangle$, to a gauge transformation. That is, we change $|\psi(s)\rangle \rightarrow |\psi'(s)\rangle = \exp(i\alpha(s))|\psi(s)\rangle$, as a consequence of which $\text{Im}\langle\psi(s)|\dot{\psi}(s)\rangle \rightarrow \text{Im}\langle\psi'(s)|\dot{\psi}'(s)\rangle = \text{Im}\langle\psi(s)|\dot{\psi}(s)\rangle + \dot{\alpha}(s)$. We then require that $\text{Im}\langle\psi'(s)|\dot{\psi}'(s)\rangle = 0$. This can be attained by taking

$$\alpha(s) = -\text{Im} \int_{s_1}^s \langle\psi(s)|\dot{\psi}(s)\rangle ds, \quad (3.6)$$

where we have assumed that $\alpha(s_1) = 0$, i.e., that $|\psi'(s_1)\rangle = |\psi(s_1)\rangle$.

The remarkable fact that $\Phi_g(C_0)$ depends only on ray-space features makes it desirable to find an expression of it that involves quantities of such a space. In order to achieve this, let us consider the operator $K(s) = \dot{\rho}(s) = d(|\psi(s)\rangle\langle\psi(s)|)/ds$. We can see that its action on $|\psi(s)\rangle$ gives

$$K(s)|\psi(s)\rangle = |\dot{\psi}(s)\rangle - \langle\psi(s)|\dot{\psi}(s)\rangle|\psi(s)\rangle. \quad (3.7)$$

$K(s)$ is invariant under a gauge transformation $|\psi(s)\rangle \rightarrow |\psi'(s)\rangle = \exp(i\alpha(s))|\psi(s)\rangle$, i.e., $K'(s) = K(s)$; hence, Eq.(3.7) holds also for the primed quantities. Let us now assume that we are dealing with a horizontal lift, that is, $\langle\psi(s)|\dot{\psi}(s)\rangle = 0$. As we have seen, this can always be achieved by a proper gauge transformation. For a horizontal lift Eq.(3.7) reduces to

$$\frac{d}{ds}|\psi(s)\rangle = \dot{\rho}(s)|\psi(s)\rangle. \quad (3.8)$$

The solution of Eq.(3.8) can be formally given as a Dyson series: $|\psi(s)\rangle = P \left(\exp \int_{s_1}^s \dot{\rho}(s) ds \right) |\psi(s_1)\rangle$. The operator P is the “parameter-ordering” operator: it rearranges a product of parameter-labeled operators such that larger parameter values are put to the left, e. g., $P(\dot{\rho}(s_1)\dot{\rho}(s_2)\dot{\rho}(s_3)) = \dot{\rho}(s_3)\dot{\rho}(s_2)\dot{\rho}(s_1)$, for $s_3 \geq s_2 \geq s_1$. Having a horizontal lift, the geometric phase reduces to $\Phi_g(C_0) = \Phi_{tot}(C_0) = \arg \langle \psi(s_1) | \psi(s_2) \rangle$. Now, $\langle \psi(s_1) | \psi(s_2) \rangle = \text{Tr}(|\psi(s_2)\rangle \langle \psi(s_1)|)$, and $|\psi(s_2)\rangle = P \left(\exp \int_{s_1}^{s_2} \dot{\rho}(s) ds \right) |\psi(s_1)\rangle$, so that we can finally write

$$\Phi_g(C_0) = \arg \text{Tr} \left\{ P \left(\exp \int_{s_1}^{s_2} \dot{\rho}(s) ds \right) \rho(s_1) \right\} \quad (3.9)$$

Eq.(3.9) gives the desired expression of $\Phi_g(C_0)$ in terms of ray-space quantities. C_0 is any smooth curve in ray-space. If C_0 is a closed curve, $\rho(s_2) = \rho(s_1)$, and $|\psi(s_2)\rangle$ must be equal to $|\psi(s_1)\rangle$ up to a phase factor: $|\psi(s_2)\rangle = e^{i\alpha} |\psi(s_1)\rangle$, with $\alpha = \arg \langle \psi(s_2) | \psi(s_1) \rangle$. For the horizontal lift we are considering, $\alpha = \arg \langle \psi(s_2) | \psi(s_1) \rangle = \Phi_g(C_0)$ and we can thus write

$$|\psi(s_2)\rangle = P \left(\exp \int_{s_1}^{s_2} \dot{\rho}(s) ds \right) |\psi(s_1)\rangle = \exp(i\Phi_g(C_0)) |\psi(s_1)\rangle. \quad (3.10)$$

3.2 Geodesics

Let us introduce now the concept of geodesics in both the Hilbert-space and the ray-space. To this end, let us refer again to Eq.(3.7). The action of $K(s)$ on $|\psi(s)\rangle$ produces a vector which is orthogonal to $|\psi(s)\rangle$, that is, $\langle \psi(s) | K(s) | \psi(s) \rangle = 0$. In general, $\langle \psi(s) | \dot{\psi}(s) \rangle \neq 0$; that is, the vector $|\dot{\psi}(s)\rangle$ tangent to the curve $C_0 = \{|\psi(s)\rangle\}$ need not be orthogonal to it. What $K(s)$ does is to produce, by acting on $|\psi(s)\rangle$, the component of $|\dot{\psi}(s)\rangle$ that is tangent to the curve C_0 . Such a component is $|\dot{\psi}(s)\rangle$ less its projection on $|\psi(s)\rangle$, i.e., $|\dot{\psi}(s)\rangle - \langle \psi(s) | \dot{\psi}(s) \rangle |\psi(s)\rangle$. Let us denote this component by $|\dot{\psi}(s)\rangle_\perp = K(s) |\psi(s)\rangle$. Under a gauge transformation $|\psi(s)\rangle \rightarrow |\psi'(s)\rangle = \exp(i\alpha(s)) |\psi(s)\rangle$ we have that $K'(s) = K(s)$, and hence it follows that $|\dot{\psi}'(s)\rangle_\perp = \exp(i\alpha(s)) |\dot{\psi}(s)\rangle_\perp$. Thus, the modulus of $|\dot{\psi}(s)\rangle_\perp$ is gauge invariant and thus constitutes an appropriate quantity to be used for a definition of extremal curves. The extremal property is defined with respect to an appropriately defined “length” of the curve. But as we want such a definition to be also parameter invariant, we need the length to be defined in terms of an integrand that is homogeneous of first degree in $|\dot{\psi}(s)\rangle$. This can be achieved if we consider the square root of the modulus and define the following functional of C_0 as the length of this curve:

$$\mathcal{L}(C_0) = \int_{s_1}^{s_2} \sqrt{\langle \dot{\psi}(s) | \dot{\psi}(s) \rangle_\perp} ds. \quad (3.11)$$

Geodesics are defined as those curves for which $\mathcal{L}(C_0)$ is extremal. By applying the tools of variational calculus it is straightforward to obtain the following differential equation:

$$\left(\frac{d}{ds} - i \langle \psi(s) | \dot{\psi}(s) \rangle \right) \frac{|\dot{\psi}(s)\rangle_\perp}{\sqrt{\langle \dot{\psi}(s) | \dot{\psi}(s) \rangle_\perp}} = f(s) |\psi(s)\rangle, \quad (3.12)$$

with $f(s)$ an arbitrary real function. Although Eq.(3.12) involves quantities that depend on some lifted curve C_0 it must be gauge and reparametrization invariant, because it follows from a quantity, Eq.(3.11), possessing such properties. We may therefore choose a different lift and parametrization to transform Eq.(3.12) according to our conveniences. We can hence choose a horizontal lift: $\langle \psi(s) | \dot{\psi}(s) \rangle = 0$, which implies that $|\dot{\psi}(s)\rangle_\perp = |\dot{\psi}(s)\rangle$ and choose the parameter s such that $\langle \dot{\psi}(s) | \dot{\psi}(s) \rangle$ is constant along C_0 . This reduces Eq.(3.12) to

$$\frac{d^2}{ds^2}|\psi(s)\rangle = \sqrt{\langle\dot{\psi}(s)|\dot{\psi}(s)\rangle}f(s)|\psi(s)\rangle \quad (3.13)$$

Now, deriving twice $\langle\psi(s)|\psi(s)\rangle = 1$ we obtain $\sqrt{\langle\dot{\psi}(s)|\dot{\psi}(s)\rangle}f(s) + \langle\dot{\psi}(s)|\dot{\psi}(s)\rangle = 0$, which fixes $f(s)$ to

$$f(s) = -\sqrt{\langle\dot{\psi}(s)|\dot{\psi}(s)\rangle}, \quad (3.14)$$

and Eq.(3.13) reads finally

$$\frac{d^2}{ds^2}|\psi(s)\rangle = -\omega^2|\psi(s)\rangle, \quad (3.15)$$

with $\omega^2 \equiv \langle\dot{\psi}(0)|\dot{\psi}(0)\rangle$. This is the equation that geodesics must satisfy, whenever they are taken as a horizontal lift from the corresponding geodesic C_0 in ray space and with the parameter s being chosen so that $\langle\dot{\psi}(s)|\dot{\psi}(s)\rangle$ is constant along the geodesic (this is called an “affine” parameter). Eq.(3.15) can be easily solved for the initial conditions $|\psi(0)\rangle = |\phi_1\rangle$ and $|\dot{\psi}(0)\rangle = \omega|\phi_2\rangle$, thus satisfying $\langle\phi_1|\phi_1\rangle = 1$, $\langle\phi_1|\phi_2\rangle = 0$, and $\langle\phi_2|\phi_2\rangle = 1$:

$$|\psi(s)\rangle = \cos(\omega s)|\phi_1\rangle + \sin(\omega s)|\phi_2\rangle. \quad (3.16)$$

An important consequence of this equation is that $\langle\psi(0)|\psi(s)\rangle = \langle\phi_1|\psi(s)\rangle = \cos(\omega s)$. Now, we can always choose a parametrization such that $\cos(\omega s) \geq 0$, for $s \in [s_1, s_2]$. Assuming that such a choice is made, $\arg\langle\psi(0)|\psi(s)\rangle = 0$. But because our lift is a horizontal one, $\arg\langle\psi(0)|\psi(s)\rangle = \Phi_g(C_0)$, so that

$$\Phi_g(C_0) = 0 \quad \text{for a geodesic } C_0. \quad (3.17)$$

From Eq.(3.16) we see that our geodesics are arcs of circles in the space whose orthonormal basis is $\{|\phi_1\rangle, |\phi_2\rangle\}$. We are thus dealing with a two-level system. A geodesic $|\psi(s)\rangle$ such as the one defined in Eq.(3.16) projects onto a geodesic in ray-space $\rho(s) = |\psi(s)\rangle\langle\psi(s)|$. Last one can be mapped onto the unit sphere in a well-known manner. Indeed, for a two-level system $\rho(s)$ has the form

$$\rho(s) = \frac{1}{2}(I + \vec{n}(s) \cdot \vec{\sigma}), \quad (3.18)$$

with $\vec{\sigma}$ being the triple of Pauli matrices, I the identity matrix, and \vec{n} a unit vector given by $\vec{n} = \text{Tr}(\rho \cdot \vec{\sigma})$.

It is therefore clear that two given (unit) vectors, $|\psi_1\rangle$ and $|\psi_2\rangle$, can always be connected by a geodesic. Indeed, we need only note that to the two vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ there correspond two unit vectors \vec{n}_1 and \vec{n}_2 lying on the unit sphere. There is always a great circle passing through two given points on the sphere. This is the geodesic arc joining ρ_1 and ρ_2 that can be lifted to a geodesic arc in Hilbert-space joining $|\psi_1\rangle$ and $|\psi_2\rangle$. If necessary, once we have this geodesic we can submit it to a gauge transformation, thereby generally destroying its horizontal but not its geodesic property.

Let us show this procedure in more detail. Consider two vectors: $|\psi_1\rangle$ and $|\psi'_2\rangle$. We take any orthonormal basis $\{|\phi_1\rangle, |\phi_2\rangle\}$ with $|\phi_1\rangle = |\psi_1\rangle$ (and $|\phi_2\rangle = (|\psi'_2\rangle - \langle\phi_1|\psi'_2\rangle)|\phi_1\rangle \left(1 - |\langle\phi_1|\psi'_2\rangle|^2\right)^{-1/2}$, though this explicit form will not be required for our present purposes). In such a basis, the general form of $|\psi'_2\rangle$, up to a global phase factor, is $|\psi_2\rangle = \cos(\theta/2)|\phi_1\rangle + e^{i\varphi}\sin(\theta/2)|\phi_2\rangle$, that is, $|\psi'_2\rangle = e^{i\alpha}|\psi_2\rangle$. We start by considering first the case in which the final vector is given by

$|\psi_2\rangle$, and then we deal with the more general case of $|\psi'_2\rangle = e^{i\alpha}|\psi_2\rangle$. The corresponding projectors $\rho_1 = |\psi_1\rangle\langle\psi_1|$ and $\rho_2 = |\psi_2\rangle\langle\psi_2|$ are given by expressions of the form of Eq.(3.18) with $\vec{n}_1 = (0, 0, 1)$ and $\vec{n}_2 = (\cos\varphi \sin\theta, \sin\varphi \sin\theta, \cos\theta)$. That means that \vec{n}_1 is the North pole (of what is called the “Bloch sphere”) and \vec{n}_2 is a point whose spherical coordinates are (θ, φ) . In order to bring \vec{n}_1 to \vec{n}_2 along a great circle we can submit it to a rotation whose axis is given by a unit vector \vec{n} parallel to $\vec{n}_1 \times \vec{n}_2$, the rotation angle being equal to θ , the angle between \vec{n}_1 and \vec{n}_2 . The unit vector \vec{n} is thus given by

$$\vec{n} = \frac{\vec{n}_1 \times \vec{n}_2}{\sin\theta}. \quad (3.19)$$

To the rotation bringing \vec{n}_1 to \vec{n}_2 it corresponds a $SU(2)$ transformation bringing $|\psi_1\rangle$ to $|\psi_2\rangle$, viz, $U(\theta, \varphi)|\psi_1\rangle = |\psi_2\rangle$, which is given by

$$U(\theta, \varphi) = \exp\left(-i\frac{\theta}{2}\vec{n} \cdot \vec{\sigma}\right) = \cos\left(\frac{\theta}{2}\right)I - i\sin\left(\frac{\theta}{2}\right)\vec{n} \cdot \vec{\sigma} = \cos\left(\frac{\theta}{2}\right)I - i\frac{\vec{n}_1 \times \vec{n}_2}{2\cos(\theta/2)} \cdot \vec{\sigma}. \quad (3.20)$$

By defining $|\psi(s)\rangle = U(\theta s, \varphi)|\phi_1\rangle$ we have that, first, $|\psi(0)\rangle = |\psi_1\rangle$, $|\psi(1)\rangle = |\psi_2\rangle$ and, second, that the curve defined by $|\psi(s)\rangle$, $s \in [0, 1]$, is a horizontal geodesic. Indeed, by explicitly writing $U(\theta s, \varphi)$ as

$$U(\theta s, \varphi) = \cos\left(\frac{\theta}{2}s\right)I - i\sin\left(\frac{\theta}{2}s\right)\vec{n}_\varphi \cdot \vec{\sigma} \quad (3.21)$$

with $\vec{n}_\varphi = (-\sin\varphi, \cos\varphi, 0)$ it is straightforward to verify that $|\psi(s)\rangle$ fulfills the defining properties of horizontal geodesics:

$$\frac{d^2}{ds^2}|\psi(s)\rangle = -\langle\dot{\psi}(s)|\dot{\psi}(s)\rangle|\psi(s)\rangle = -\frac{\theta^2}{4}|\psi(s)\rangle, \quad (3.22)$$

$$\langle\psi(s)|\dot{\psi}(s)\rangle = 0. \quad (3.23)$$

Hence, for $|\psi_1\rangle = |\phi_1\rangle$ and $|\psi_2\rangle = \cos(\theta/2)|\phi_1\rangle + e^{i\varphi}\sin(\theta/2)|\phi_2\rangle$ we have proved that there is a horizontal geodesic joining them, which is given by $|\psi(s)\rangle = U(\theta s, \varphi)|\phi_1\rangle$, with $U(\theta s, \varphi)$ as in Eq.(3.21). Next, let us consider a general final vector $|\psi'_2\rangle = e^{i\alpha}|\psi_2\rangle$. In this case we need only change $U(\theta s, \varphi)$ by $e^{-i\alpha s}U(\theta s, \varphi)$ and the curve $|\psi'(s)\rangle = e^{-i\alpha s}U(\theta s, \varphi)|\phi_1\rangle$, with $|\psi'(0)\rangle = |\psi_1\rangle$, $|\psi'(1)\rangle = |\psi'_2\rangle$, will still be a geodesic; that is, it satisfies Eq.(3.12) (with $f(s) = \theta/2$) though it is no longer a horizontal one ($\langle\psi'(s)|\dot{\psi}'(s)\rangle = -i\alpha$).

In summary, we have proved that any two vectors, $|\psi_1\rangle$ and $|\psi_2\rangle$, can be connected by a geodesic \mathcal{C}_0 . If this geodesic happens to be a horizontal one, then its dynamical phase vanishes and so does its total phase $\arg\langle\psi_1|\psi_2\rangle$, as follows from Eq.(3.16). Hence, the geometric phase $\Phi_g(C_0) = 0$. This last property is gauge independent and so holds true for any lift. However, if the geodesic \mathcal{C}_0 is not horizontal, then $\Phi_{dyn}(C_0) \neq 0$ and so also $\arg\langle\psi_1|\psi_2\rangle \neq 0$, though $\Phi_g(C_0) = 0$.

We note that irrespective of the dimensionality of the Hilbert space to which $|\psi_1\rangle$ and $|\psi_2\rangle$ belong, the only tools we have used to show how they can be joined by a geodesic are those of a two-level system. This is because there were only two vectors involved and we could thus restrict ourselves to work on a two-dimensional subspace of the whole Hilbert space. Now, the fact that any two unit vectors can always be connected by a geodesic leads to an alternative formulation of the geometric phase. It rests upon the concept of Bargmann invariants, that we shall present next. Eq.(3.17) will play a central role, together with quantities like $\arg\langle\psi_1|\psi_2\rangle$. When the total

phase $\arg\langle\psi_1|\psi_2\rangle = 0$ we say that $|\psi_1\rangle$ and $|\psi_2\rangle$ are “in phase”. As we have seen, this is the case when these vectors can be joined by a horizontal geodesic. Consider a third vector $|\psi_3\rangle$ that is joined to $|\psi_2\rangle$ by a *horizontal* geodesic and hence $\arg\langle\psi_2|\psi_3\rangle = 0$ as well. Our three vectors are thus joined by a curve conformed by two arcs, each one being a horizontal geodesic. Can we conclude that the total phase between $|\psi_3\rangle$ and $|\psi_1\rangle$ vanishes too? The answer is generally on the negative. Being “in phase” is not a transitive property. The following discussion will illustrate this point.

3.3 Bargmann invariants

Let us take N points in ray-space: $\rho_1, \rho_2, \dots, \rho_N$. As we have just seen, each pair of these points can be connected by a geodesic arc. Let us denote by C_0 the curve formed by the $N - 1$ geodesic arcs joining the N points. Let us assume that any two successive pairs of the points are non-orthogonal. That is, choosing any lift of them, $|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_N\rangle$, all inner products $\langle\psi_i|\psi_{i+1}\rangle \neq 0$, for $i = 1, \dots, N - 1$. Let us calculate $\Phi_g(C_0)$. It is given by

$$\Phi_g(C_0) = \Phi_{tot}(C_0) - \Phi_{dyn}(C_0) = \arg\langle\psi_1|\psi_N\rangle - \sum_{k=1}^{N-1} \Phi_{dyn}^{(k,k+1)}, \quad (3.24)$$

where $\Phi_{dyn}^{(k,k+1)}$ is the dynamical phase for the geodesic joining $|\psi_k\rangle$ with $|\psi_{k+1}\rangle$. But, because $\Phi_g^{(k,k+1)} = 0$, we can write $\Phi_{dyn}^{(k,k+1)} = \Phi_{tot}^{(k,k+1)} - \Phi_g^{(k,k+1)} = \arg\langle\psi_k|\psi_{k+1}\rangle$. Now, $\sum_{k=1}^{N-1} \arg\langle\psi_k|\psi_{k+1}\rangle = \arg\prod_{k=1}^{N-1} \langle\psi_k|\psi_{k+1}\rangle$, and $\arg\langle\psi_1|\psi_N\rangle = -\arg\langle\psi_N|\psi_1\rangle$, so that

$$\Phi_g(C_0) = \arg\langle\psi_1|\psi_N\rangle - \arg\prod_{k=1}^{N-1} \langle\psi_k|\psi_{k+1}\rangle = -\arg\left(\prod_{k=1}^{N-1} \langle\psi_k|\psi_{k+1}\rangle\right) \langle\psi_N|\psi_1\rangle \quad (3.25)$$

and we can write

$$\Phi_g(C_0) = -\arg\langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_3\rangle\cdots\langle\psi_N|\psi_1\rangle. \quad (3.26)$$

Although this expression for $\Phi_g(C_0)$ has been derived by joining $|\psi_1\rangle, \dots, |\psi_N\rangle$ with a series of geodesic arcs that all together make up C_0 , the final expression contains nothing but the points $|\psi_1\rangle, \dots, |\psi_N\rangle$ themselves. Such a result brings strikingly to the fore the topological character of the geometric phase. Quantities like $\langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_3\rangle\langle\psi_3|\psi_1\rangle$ are called “Bargmann invariants”. They generalize $|\langle\psi_1|\psi_2\rangle|^2$, which is invariant under simultaneous $U(1)$ (gauge) transformations of its constituent parties: $|\psi_1\rangle \rightarrow |\psi'_1\rangle = \exp(i\alpha_1)|\psi_1\rangle$, $|\psi_2\rangle \rightarrow |\psi'_2\rangle = \exp(i\alpha_2)|\psi_2\rangle$. Quantities that are invariant under $U(1) \otimes U(1) \otimes \dots$ were introduced by Bargmann for studying the difference between unitary and anti-unitary transformations [11].

The curve C_0 in Eq.(3.25) was assumed to be open, as $\rho_N \neq \rho_1$. However, we can have a closed curve \tilde{C}_0 by completing the $N - 1$ -sided polygon C_0 with a geodesic arc that connects ρ_N with ρ_1 . By repeating the above steps that led us to Eq.(3.25), though taking into account that now $\Phi_{tot}(\tilde{C}_0) = 0$ because the final point $\psi_{N+1} = \psi_1$, we see that $\Phi_g(\tilde{C}_0) = -\Phi_{dyn}(\tilde{C}_0) = -\arg\prod_{k=1}^N \langle\psi_k|\psi_{k+1}\rangle$, so that $\Phi_g(\tilde{C}_0)$ is given by just the same expression as in Eq.(3.26). In other words, $\Phi_g(\tilde{C}_0) = \Phi_g(C_0)$: both \tilde{C}_0 and C_0 have the same geometric phase.

Starting from Eq.(3.26) it is possible to recover the results previously found for general open curves [8]. One proceeds by approximating a given curve by a polygonal arc made up of $N \rightarrow \infty$ geodesic arcs. By a limiting procedure one recovers then $\Phi_g(C_0) = \Phi_{tot}(C_0) - \Phi_{dyn}(C_0)$ with

$\Phi_{tot}(\mathcal{C}_0)$ and $\Phi_{dyn}(\mathcal{C}_0)$ given by Eqs.(3.3) and (3.4), respectively. Also Eq.(3.9) can be recovered in a similar fashion [8].

Coming back to Eq.(3.26), let us denote the N -vertex invariant of the right-hand side as

$$\Delta^{(N)}(\psi_1, \dots, \psi_N) = \langle \psi_1 | \psi_2 \rangle \langle \psi_2 | \psi_3 \rangle \dots \langle \psi_N | \psi_1 \rangle. \quad (3.27)$$

We can prove by induction that it can be expressed in terms of the (fundamental) three-vertex invariant as

$$\arg \Delta^{(N)}(\psi_1, \dots, \psi_N) = \sum_{k=2}^{N-1} \arg \Delta^{(3)}(\psi_1, \psi_k, \psi_{k+1}). \quad (3.28)$$

This result is suggested by considering the N -vertex invariant as represented by an N -sided polygon and then subdividing this polygon into $N - 2$ triangles. For example, for $N = 4$ such a triangulation – which adds a line connecting the vertices 1 and 3 – suggests that we insert in the expression for $\Delta^{(4)}(\psi_1, \dots, \psi_4)$ the quantity $\langle \psi_3 | \psi_1 \rangle \langle \psi_1 | \psi_3 \rangle$ which does not alter its argument because it is real and positive:

$$\begin{aligned} \arg \Delta^{(4)}(\psi_1, \dots, \psi_4) &= \arg (\langle \psi_1 | \psi_2 \rangle \langle \psi_2 | \psi_3 \rangle \langle \psi_3 | \psi_4 \rangle \langle \psi_4 | \psi_1 \rangle \times \langle \psi_3 | \psi_1 \rangle \langle \psi_1 | \psi_3 \rangle) \\ &= \arg \langle \psi_1 | \psi_2 \rangle \langle \psi_2 | \psi_3 \rangle \langle \psi_3 | \psi_1 \rangle + \arg \langle \psi_1 | \psi_3 \rangle \langle \psi_3 | \psi_4 \rangle \langle \psi_4 | \psi_1 \rangle \\ &= \Delta^{(3)}(\psi_1, \psi_2, \psi_3) + \Delta^{(3)}(\psi_1, \psi_3, \psi_4). \end{aligned}$$

It is then clear how this result generalizes to Eq.(3.28). The triangulations leading to the additive property expressed by Eq.(3.28) suggest also that $\arg \Delta^{(N)}$ has the nature of an “area”. It can be shown, indeed, that Φ_g can generally be expressed as a (two-dimensional) surface integral of a two-form [8].

Let us consider the concrete case of a two-level system and calculate $\Delta^{(3)}(\psi_1, \psi_2, \psi_3)$. We can write this Bargmann invariant in the form

$$\Delta^{(3)}(\psi_1, \psi_2, \psi_3) = \langle \psi_1 | \psi_2 \rangle \langle \psi_2 | \psi_3 \rangle \langle \psi_3 | \psi_1 \rangle = \langle \psi_1 | \rho_2 \rho_3 | \psi_1 \rangle \quad (3.29)$$

$$= \text{Tr} [|\psi_1\rangle \langle \psi_1| \rho_2 \rho_3] = \text{Tr} [\rho_1 \rho_2 \rho_3]. \quad (3.30)$$

For two-level systems, $\rho_i = (I + \vec{n}_i \cdot \vec{\sigma})/2$, $i = 1, 2, 3$. A straightforward calculation gives

$$\text{Tr} [\rho_1 \rho_2 \rho_3] = \frac{1}{4} [1 + \vec{n}_1 \cdot \vec{n}_2 + \vec{n}_2 \cdot \vec{n}_3 + \vec{n}_3 \cdot \vec{n}_1 + i \vec{n}_1 \cdot (\vec{n}_2 \times \vec{n}_3)]. \quad (3.31)$$

Now it is easy to obtain the phase χ of $\Delta^{(3)}(\psi_1, \psi_2, \psi_3)$, as we have the real and imaginary parts of this last quantity. Denoting by θ_{jk} the angle between \vec{n}_j and \vec{n}_k , i.e., $\cos \theta_{jk} = \vec{n}_j \cdot \vec{n}_k$, we obtain from Eq.(3.31) that

$$\cos \chi = \frac{\cos^2 (\theta_{12}/2) + \cos^2 (\theta_{23}/2) + \cos^2 (\theta_{31}/2) - 1}{2 \cos (\theta_{12}/2) \cos (\theta_{23}/2) \cos (\theta_{31}/2)}, \quad (3.32)$$

which is a well-known expression for the cosine of half the solid angle of the spherical triangle whose vertices are \vec{n}_1 , \vec{n}_2 , \vec{n}_3 . This means that χ is just half the solid angle subtended by the three points representing the states $|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi_3\rangle$ on the (Bloch) sphere. This is a central result in the theory of Berry phases and constitutes a special case of what we have derived before, namely Eq.(2.50) with $k = 1/2$, as it corresponds for spin-1/2 particles.

Chapter 4

Pancharatnam's phase and its measurement by polarimetry and interferometry

We have introduced the total phase between two states as $\arg\langle\psi_1|\psi_2\rangle$. This constitutes a generalization of Pancharatnam's definition for the relative phase between two polarization states of light. Pancharatnam [3] addressed the problem of how to decide whether two nonorthogonal polarization states could be said to be “in phase”. His proposal was based on the following operational prescription. Consider two non-orthogonal polarization states, $|i\rangle$ and $|f\rangle$, with $|i\rangle \neq |f\rangle$ and let them interfere with one another. Apply a phase-shift ϕ to one of the states. The resulting intensity pattern is given by

$$I = |e^{i\phi}|i\rangle + |f\rangle|^2 = 2 + 2|\langle i|f\rangle|\cos(\phi - \arg\langle i|f\rangle). \quad (4.1)$$

Find now ϕ for which I is maximum. This occurs for $\phi = \arg\langle i|f\rangle \equiv \Phi_{tot}$, which is thereby defined as the total (or Pancharatnam) phase between $|i\rangle$ and $|f\rangle$. If $\arg\langle i|f\rangle = 0$ the states are said to be in phase. Polarization states are two-level systems. When they are submitted to the action of intensity-preserving optical elements, like wave-plates, then the corresponding polarization transformations belong to the group $U(2)$, or to the group $SU(2)$, if global phase factors are left aside. We can exhibit Φ_{tot} by submitting an initial state $|i\rangle$ to an arbitrary transformation $U \in SU(2)$ that brings it into a final state $|f\rangle = U|i\rangle$. The intensity measurement for which Eq.(4.1) applies can be implemented with, say, a Mach-Zehnder interferometer. Alternatively, one could employ polarimetric methods. We will discuss both methods in what follows. But before that, it will be useful to say some few words about the different parametrizations used for writing the elements of $SU(2)$.

As we saw before, a parametrization of $U \in SU(2)$, when viewed as realizing a rotation by an angle α around an axis $\hat{n} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\varphi)$, is given by

$$U(\alpha, \theta, \varphi) = \exp\left[i\frac{\alpha}{2}\hat{n} \cdot \vec{\sigma}\right]. \quad (4.2)$$

In this case U is specified by the three parameters $(\alpha, \theta, \varphi)$. Alternatively, we could specify U by so-called Euler parameters:

$$U(\xi, \eta, \zeta) = \exp\left(-i\frac{\xi}{2}\sigma_y\right)\exp\left(i\frac{\eta}{2}\sigma_z\right)\exp\left(-i\frac{\zeta}{2}\sigma_y\right), \quad (4.3)$$

which we call the YZY -form for obvious reasons. It corresponds to three rotations around Cartesian axes \hat{e}_y and \hat{e}_z . Another useful form of U , the ZYZ -form, is given by

$$U(\beta, \gamma, \delta) = \exp\left(i\left(\frac{\delta + \gamma}{2}\right)\sigma_z\right) \exp(-i\beta\sigma_y) \exp\left(i\left(\frac{\delta - \gamma}{2}\right)\sigma_z\right) = \begin{pmatrix} e^{i\delta} \cos \beta & -e^{i\gamma} \sin \beta \\ e^{-i\gamma} \sin \beta & e^{-i\delta} \cos \beta \end{pmatrix}. \quad (4.4)$$

The representation given by Eq.(4.4) is particularly useful for exhibiting Pancharatnam's phase. Indeed, taking as initial state $|i\rangle = |+\rangle_z$, the eigenstate of σ_z for the eigenvalue $+1$, and setting $|f\rangle = U|+\rangle_z$ we obtain

$$\langle i|f\rangle = {}_z\langle +|U(\beta, \gamma, \delta)|+\rangle_z = e^{i\delta} \cos \beta. \quad (4.5)$$

Thus, $\Phi_{tot} = \arg \langle i|f\rangle = \delta + \arg(\cos \beta)$, for $\beta \neq (2n+1)\pi/2$. Because $\cos \beta$ can take on positive and negative real values, $\arg(\cos \beta)$ equals 0 or π , and Φ_{tot} is thus defined modulo π . The parametrization of Eq.(4.4) gives therefore $\Phi_{tot} = \delta$ (modulo π). On the other hand, for the optical implementation of U another parametrization is more appropriate. It is well known that we can implement any $U \in SU(2)$ with the help of three retarders, two quarter-wave plates and one half-wave plate [19, 20]. In polarization-space of, e.g., horizontally and vertically polarized states of light, $\{|H\rangle, |V\rangle\}$, U is best represented in the form given by Eq.(4.3), the YZY -form, because of the following relationship involving the Euler angles $\alpha_1, \alpha_2, \alpha_3$:

$$\exp(-i(\alpha_3 + 3\pi/4)\sigma_y) \exp(i(\alpha_1 - 2\alpha_2 + \alpha_3)\sigma_z) \exp(i(\alpha_1 - \pi/4)\sigma_y) = Q(\alpha_3)H(\alpha_2)Q(\alpha_1). \quad (4.6)$$

Here, Q means a quarter-wave plate and H a half-wave plate. The arguments of these retarders are the angles of their major axes to the vertical direction. In the case of the U given by Eq.(4.3), by applying Eq.(4.6) we obtain

$$U(\xi, \eta, \zeta) = Q\left(\frac{-3\pi + 2\xi}{4}\right) H\left(\frac{\xi - \eta - \zeta - \pi}{4}\right) Q\left(\frac{\pi - 2\zeta}{4}\right). \quad (4.7)$$

Having seen the different parametrizations which are relevant for our purposes, let us turn now to discuss the implementation of some experimental arrangements that exhibit Pancharatnam's phase.

4.1 Interferometric arrangement

In general, with an interferometric array Pancharatnam's phase can be obtained from intensity measurements that are described by Eq.(4.1). Introducing U from Eq.(4.3) into Eq.(4.1) we obtain

$$\begin{aligned} I &= \left| \frac{1}{\sqrt{2}} (e^{i\phi} |+\rangle_z + U(\xi, \eta, \zeta) |+\rangle_z) \right|^2 = \\ &= 1 - \cos\left(\frac{\eta}{2}\right) \cos\left(\frac{\xi + \zeta}{2}\right) \cos(\phi) - \sin\left(\frac{\eta}{2}\right) \cos\left(\frac{\xi - \zeta}{2}\right) \sin(\phi). \end{aligned} \quad (4.8)$$

From Eqs.(4.3,4.4) we derive the following relationship for the parameters of these two representations:

$$\tan(\delta) = \tan\left(\frac{\eta}{2}\right) \frac{\cos\left(\frac{\xi-\zeta}{2}\right)}{\cos\left(\frac{\xi+\zeta}{2}\right)}. \quad (4.9)$$

Hence, I can be written as

$$I = 1 - \cos\left(\frac{\eta}{2}\right) \cos\left(\frac{\xi+\zeta}{2}\right) \sec(\delta) \cos(\delta - \phi), \quad (4.10)$$

making it evident that an interferometric method for exhibiting Φ_{tot} would require measuring the shift induced by U on the intensity pattern by an angle $\delta = \Phi_{tot}$ (modulo π). Now, the expression for I as given in Eq.(4.10) mixes δ with parameters of a representation to which it does not belong. By converting Eq.(4.10) to the representation $U(\beta, \gamma, \delta)$ we obtain

$$I = 1 - \cos(\beta) \cos(\delta - \phi). \quad (4.11)$$

The visibility $v \equiv (I_{\max} - I_{\min}) / (I_{\max} + I_{\min})$ is thus given by $v = \cos \beta$. It is independent of Pancharatnam's phase. In terms of the parameters ξ, η, ζ the visibility is given by

$$v^2(\xi, \eta, \zeta) = \frac{1}{2} [1 + \cos \xi \cos \zeta - \cos \eta \sin \xi \sin \zeta]. \quad (4.12)$$

For comparison with experimental tests, it is useful to write v^2 in terms of the retarders' angles:

$$\begin{aligned} v^2(\alpha_1, \alpha_2, \alpha_3) &= \\ &= \frac{1}{2} \left[1 + \cos\left(\frac{3\pi + 4\alpha_3}{2}\right) \cos\left(\frac{\pi - 4\alpha_1}{2}\right) - \cos(2\alpha_1 - 4\alpha_2 + 2\alpha_3) \sin\left(\frac{3\pi + 4\alpha_3}{2}\right) \sin\left(\frac{\pi - 4\alpha_1}{2}\right) \right]. \end{aligned}$$

Let us now refer specifically to a Mach-Zehnder interferometer. Our initial state is taken to be the vertically polarized state $|V\rangle$ that enters the first beam-splitter (see Fig.(7.1)) along the X -direction. A straightforward calculation yields for the intensity measured at one of the output channels:

$$I_V = \frac{1}{2} \left[1 - \cos\left(\frac{\eta}{2}\right) \cos\left(\frac{\xi+\zeta}{2}\right) \cos(\phi) - \sin\left(\frac{\eta}{2}\right) \cos\left(\frac{\xi-\zeta}{2}\right) \sin(\phi) \right]. \quad (4.13)$$

This can also be written as

$$I_V = \frac{1}{2} [1 - \cos(\beta) \cos(\phi - \delta)]. \quad (4.14)$$

The above result suggest a direct measurement of Pancharatnam's phase $\delta = \Phi_{tot}$ (modulo π) by recording the fringe-shift between two interferograms, one of them serving as a reference ($\delta = 0$), and the other being obtained after applying the U transformation. There is however a practical problem with this method. An interferometric array is very sensitive to minute changes of its components, making it very difficult to accurately measuring δ . Different strategies are usually applied to overcome these shortcomings. Mechanical and thermal isolation of the arrangement is the most direct one, but measurements are then rather awkward. Damping instabilities by a feedback mechanism is another possibility; but it makes the arrangement more involved and difficult to operate.

Recently, a novel strategy has been employed [23] with a Mach-Zehnder array. It was based on the following observation. Eq.(4.14) holds for an initial state that is vertically polarized. When the initial state is instead horizontally polarized, then the intensity is given by

$$I_H = \frac{1}{2} [1 - \cos(\beta) \cos(\phi + \delta)]. \quad (4.15)$$

We observe that intensities I_V and I_H are shifted with respect to each other by 2δ , and this can be exploited for measuring δ . To this end, one polarizes one half - say the upper half - of the laser beam vertically, and the lower half horizontally. With such a beam one feeds the interferometer, so that one can capture at the output an interferogram, half of which corresponds to I_V and the other half to I_H . The upper and lower fringes will show a relative shift of 2δ . As both halves come from the same beam, they will be equally affected by whatever perturbations. The array is therefore insensitive to instabilities. One thus needs only to accurately measure the relative fringe-shift in each interferogram in order to obtain δ . Fig.(7.1) shows an sketch of the interferometric arrangement. By applying this method Pancharatnam's phase could be measured with an accuracy that is similar to the one reached by the polarimetric method. Experimental results are shown in Fig.(7.4) for $\cos^2 \Phi_{tot}$. The versatility of the arrangement was also tested by measuring the visibility and comparing these results with the theoretical predictions given above for $v^2(\alpha_1, \alpha_2, \alpha_3)$ (see Fig.(7.6)).

4.2 Polarimetric arrangement

Wagh and Rakhecha proposed some years ago [12, 13] a polarimetric method to measure Pancharatnam's phase. Such a method is experimentally more difficult to implement than the interferometric method; but it was considered the more accurate of the two, because it requires a single beam. Both methods were tested in experiments performed with neutrons [14, 15], whose spins were subjected to $SU(2)$ transformations through the action of a magnetic field. The conclusion was that polarimetry was inherently superior to interferometry, because of the aforementioned instabilities of the latter, where two beams are involved. Now, it is not obvious that one can extract phase information from a single beam. However, as we shall see, polarimetry in the present case can be understood as "virtual interferometry".

Consider an initial, polarized state $|i\rangle = |+\rangle_z$ that is submitted to a $\pi/2$ -rotation around an axis perpendicular to the polarization axis (z), e.g., a rotation around the x -axis. This produces the state $(|+\rangle_z - i|-\rangle_z)/\sqrt{2}$. Applying then to this state the operator $\exp(-i\phi\sigma_z/2)$ we obtain the state $V|+\rangle_z \equiv \exp(-i\phi\sigma_z/2)\exp(-i\pi\sigma_x/4)|+\rangle_z = (e^{-i\phi/2}|+\rangle_z - ie^{i\phi/2}|-\rangle_z)/\sqrt{2} = e^{-i\phi/2}(|+\rangle_z - ie^{i\phi}|-\rangle_z)/\sqrt{2}$. We have thus generated a relative phase-shift ϕ between $|+\rangle_z$ and $|-\rangle_z$. This is analogous to what is achieved in an interferometer by a relative change in the length of the two optical paths. We apply then a $U \in SU(2)$ and obtain the state $UV|+\rangle_z = (e^{-i\phi/2}U|+\rangle_z - ie^{i\phi/2}U|-\rangle_z)/\sqrt{2} \equiv |\chi_+\rangle + |\chi_-\rangle$. From this last state we can extract Pancharatnam's phase. To this end, we project $|\chi_+\rangle + |\chi_-\rangle$ on the state $V|+\rangle_z$. The corresponding intensity is given by

$$I = |{}_z\langle + | V^\dagger (|\chi_+\rangle + |\chi_-\rangle)|^2. \quad (4.16)$$

Let us write $V|+\rangle_z = (e^{-i\phi/2}|+\rangle_z - ie^{i\phi/2}|-\rangle_z)/\sqrt{2} \equiv |\varphi_+\rangle + |\varphi_-\rangle$ and take U as given by $U(\beta, \gamma, \delta)$ of Eq.(4.4). Calculating the amplitude ${}_z\langle + | V^\dagger (|\chi_+\rangle + |\chi_-\rangle) = (\langle\varphi_+| + \langle\varphi_-|)(|\chi_+\rangle + |\chi_-\rangle)$ we obtain, using $\langle\varphi_\pm|\chi_\pm\rangle = \exp(\pm i\delta)\cos(\beta)/2$, and $\langle\varphi_\mp|\chi_\pm\rangle = i\exp(\mp i(\gamma + \phi))\sin(\beta)/2$, that $(\langle\varphi_+| + \langle\varphi_-|)(|\chi_+\rangle + |\chi_-\rangle) = \cos(\beta)\cos(\delta) + i\sin(\beta)\cos(\gamma + \phi)$ and, hence, that the intensity amounts to

$$I = \cos^2(\beta)\cos^2(\delta) + \sin^2(\beta)\cos^2(\gamma + \phi). \quad (4.17)$$

Eq.(4.17) contains Pancharatnam's phase $\delta = \Phi_{tot}$ so that it can be extracted through intensity measurements. Indeed, we observe from Eq.(4.17) that the minimal and maximal intensities are given by $I_{\min} = \cos^2(\beta) \cos^2(\delta)$ and $I_{\max} = \cos^2(\beta) \cos^2(\delta) + \sin^2(\beta)$, respectively, so that

$$\cos^2(\delta) = \frac{I_{\min}}{1 - I_{\max} + I_{\min}}. \quad (4.18)$$

A concrete optical arrangement requires that we implement V and U with retarders. To begin with, $\exp(-i\pi\sigma_x/4) = Q(\frac{\pi}{4})$ and $\exp(-i\phi\sigma_z/2) = Q(\frac{\pi}{4})H(\frac{\phi-\pi}{4})Q(\frac{\pi}{4})$. Using $Q^2(\frac{\pi}{4}) = H(\frac{\pi}{4})$ and $\exp(+i\phi\sigma_z/2) = Q(-\frac{\pi}{4})H(\frac{\phi+\pi}{4})Q(-\frac{\pi}{4})$ we obtain

$$U_{tot} \equiv V^\dagger UV = H\left(-\frac{\pi}{4}\right) H\left(\frac{\phi+\pi}{4}\right) Q\left(-\frac{\pi}{4}\right) U Q\left(\frac{\pi}{4}\right) H\left(\frac{\phi-\pi}{4}\right) H\left(\frac{\pi}{4}\right). \quad (4.19)$$

As for U , it is convenient to employ the form $U(\xi, \eta, \zeta)$ of Eq.(4.3). This form can be directly implemented with retarders according to Eq.(4.7), i.e., in the form QHQ . Inserting this QHQ for U into Eq.(4.19) we end up requiring nine wave plates. In order to reduce this number as much as possible we apply relations like $Q(\alpha)H(\beta) = H(\beta)Q(2\beta - \alpha)$, $Q(\alpha)H(\beta)H(\gamma) = Q(\alpha + \pi/2)H(\alpha - \beta + \gamma - \pi/2)$, and similar ones [21]. After this, we obtain an array of five retarders:

$$\begin{aligned} U_{tot} = & Q\left(-\frac{3\pi}{4} - \frac{\phi}{2}\right) Q\left(-\frac{5\pi+2\xi}{4} - \frac{\phi}{2}\right) Q\left(-\frac{9\pi+2(\xi+\eta)}{4} - \frac{\phi}{2}\right) \times \\ & \times H\left(-\frac{7\pi+\xi+\eta-\zeta}{4} - \frac{\phi}{2}\right) Q\left(-\frac{\pi}{4} - \frac{\phi}{2}\right). \end{aligned} \quad (4.20)$$

Note that such an arrangement could be implemented by mounting the five plates having a common rotation axis, so that all the plates can be rotated simultaneously by the same angle $\phi/2$. The intensity to be measured is given by the following expression:

$$\begin{aligned} I &= |{}_z\langle + | U_{tot} | + \rangle_z|^2 = \\ &= \cos^2\left(\frac{\eta}{2}\right) \cos^2\left(\frac{\xi+\zeta}{2}\right) + \left[\cos\left(\frac{\eta}{2}\right) \sin\left(\frac{\xi+\zeta}{2}\right) \cos(\phi) + \sin\left(\frac{\eta}{2}\right) \sin\left(\frac{\xi-\zeta}{2}\right) \sin(\phi) \right]^2. \end{aligned} \quad (4.21)$$

From this intensity we extract Pancharatnam's phase, as given by Eq.(4.18). This theoretical prediction have been tested under different conditions [23]. Thus, by fixing ζ to 2π , so that $\cos^2(\delta) = I_{\min} (1 - I_{\max} + I_{\min})^{-1} = \cos^2(\eta/2)$ for all ξ , Pancharatnam's phase $\Phi_{tot} = \eta/2$. With $\zeta = 2\pi$ the arrangement that realizes the corresponding U_{tot} reduces to

$$U_{tot}^{\zeta=2\pi} = Q(\phi) Q\left(-\frac{\xi}{2} + \phi\right) H\left(\frac{\eta-\xi}{4} + \phi\right), \quad (4.22)$$

in which the rotation angle ϕ has been redefined according to $(-3\pi - 2\phi)/4 \rightarrow \phi$. Experimental results are shown in Fig.(7.5).

If instead $\xi = -\pi$, it still holds that $\cos^2(\delta) = I_{\min} (1 - I_{\max} + I_{\min})^{-1} = \cos^2(\eta/2)$, this time for all ζ , so that $\Phi_{tot} = \eta/2$, as before. The corresponding arrangement is now given by

$$U_{tot}^{\xi=-\pi} = Q\left(\frac{3\pi+2\eta-2\phi}{4}\right) H\left(\frac{-4\pi+\zeta+\eta-2\phi}{4}\right) Q\left(\frac{-\pi-2\phi}{4}\right). \quad (4.23)$$

The full arrangement of five wave-plates was also implemented as shown in Fig.(7.2) and the results confirmed theoretical predictions with the expected accuracy, as also shown in Fig.(7.5). Though all these experiments were performed with a cw He-Ne laser an alternative setting using single-photon sources should produce similar results. This is because all predictions under study rest on topological rather than on quantum-mechanical features.

Chapter 5

Geometric phase for mixed states

The geometric phase has been introduced as a feature that involves projectors $\rho = |\psi\rangle\langle\psi|$. i.e., pure states. It is natural to ask whether a similar concept can be defined for mixed states. The answer is that it is indeed possible to do this, as was shown by Uhlmann [17], who based his approach on the concept of parallel transport. When $|\psi(s)\rangle$ evolves in some parameter space under parallel transport it does it by remaining in-phase with its infinitesimally neighboring state $|\psi(s+ds)\rangle$. We say that under parallel transport the system does not suffer local phase changes. However, after completing a closed loop a state may have acquired a nontrivial phase, which can be traced back to the curvature of the parameter space. This notion can be extended to systems being in mixed states. To this end, Uhlmann considered a so-called “purification” of the system being in a mixed state into a system being in a pure state. That is, one considers the mixed state as corresponding to a subsystem of a larger system which is in a pure state. There are infinitely many possible purifications of a given mixed state. Thus, a cyclic evolution of the latter induces infinitely many evolutions of the purified systems. However, one of these evolutions can be singled out as the one which is maximally parallel. This leads to a definition of geometric phases for mixed states.

An alternative approach was addressed more recently by Sjöqvist *et al.* [18]. It is more physically motivated than Uhlmann’s, but like this one it rests on connecting the mixed system to pure systems. The starting point is Pancharatnam’s approach to the total phase. Let us remind that in this approach one considers the interference of two states. One of them, the initial state $|i\rangle$, is the reference state to which a phase-shift ϕ is applied. This state interferes with a state $|f\rangle = U|i\rangle$, with U being a unitary operator. The interference pattern is given by Eq.(4.1), that we re-write here as

$$I = |e^{i\phi}|i\rangle + U|i\rangle|^2 = 2 + 2|\langle i|U|i\rangle| \cos(\phi - \arg\langle i|U|i\rangle) = 2 + 2v \cos(\phi - \Phi_{tot}), \quad (5.1)$$

with $v = |\langle i|U|i\rangle|$ the visibility and $\Phi_{tot} = \arg\langle i|U|i\rangle$ the total phase between $|i\rangle$ and $|f\rangle = U|i\rangle$.

Consider now a mixed state $\rho = \sum_i w_i |i\rangle\langle i|$, with $\sum_i w_i = 1$. The intensity profile will now be given by the contributions of all individual pure states that conform the mixed state ρ :

$$I = \sum_i w_i |e^{i\phi}|i\rangle + U|i\rangle|^2 = 2 + 2 \sum_i w_i |\langle i|U|i\rangle| \cos(\phi - \arg\langle i|U|i\rangle). \quad (5.2)$$

We can write I in a basis-independent form as

$$I = 2 + 2|Tr(U\rho)| \cos[\phi - \arg Tr(U\rho)]. \quad (5.3)$$

It is then clear that the visibility is now given by $v = |\text{Tr}(U\rho)|$ and that the total phase can be operationally defined as $\Phi_{tot} = \arg \text{Tr}(U\rho)$, which is the value of the shift ϕ at which the maximal intensity is attained. Of course, such a definition reduces to Pancharatnam's original definition for a pure state $\rho = |i\rangle\langle i|$.

The above definition assumes a unitary evolution $|i\rangle \rightarrow |f\rangle = U|i\rangle$. A non-unitary evolution can be handled by modeling it with the help of an environment being in a pure state $|0_e\rangle\langle 0_e|$ that is appended to the given mixed state. The system plus environment is then described by $\tilde{\rho} = \rho \otimes |0_e\rangle\langle 0_e|$ and evolves unitarily $\tilde{\rho} \rightarrow \tilde{\rho}' = U\tilde{\rho}U^\dagger$ in such a way that by tracing over the environment we recover the given change of the mixed state: $\rho \rightarrow \rho' = \text{Tr}_e \tilde{\rho}'$. Introducing an orthonormal basis $\{|k_e\rangle\}_{k=0,\dots,M}$ for the environment, we can write $\text{Tr}_e \tilde{\rho}' = \sum_k K_k \rho K_k^\dagger$, with $K_k \equiv \langle k_e|U|0_e\rangle$ being the so-called Kraus operators. The map $\rho \rightarrow \rho'$ is thus a completely positive map that takes density operators into density operators.

Let us turn back to unitary evolutions. We have extended Pancharatnam's phase to unitarily evolving mixed states. Now let us address a similar extension of the geometric phase. The unitary evolution we have in sight is of the form $\rho(s) = U(s) \rho_0 U^\dagger(s)$. For pure states $|\psi(s)\rangle$ the geometric phase was equal to the total phase for a state undergoing parallel evolution: $\langle \psi(s)|\dot{\psi}(s)\rangle = 0$. In that case the dynamical phase vanishes. We should then try to extend the notion of parallel transport for mixed states. For such an evolution the state $\rho(s)$ should be in phase with the state infinitesimally near to it, $\rho(s+ds) = U(s+ds) \rho_0 U^\dagger(s+ds) = U(s+ds) U^\dagger(s) \rho(s) U(s) U^\dagger(s+ds)$. According to our previous definition, the phase difference between $\rho(s)$ and $\rho(s+ds)$ is given by $\arg \text{Tr}(U(s+ds) U^\dagger(s) \rho(s))$ in this case. For $\rho(s)$ and $\rho(s+ds)$ to be in phase then, $\arg \text{Tr}(U(s+ds) U^\dagger(s) \rho(s))$ should vanish. However, because $\text{Tr}(\rho(s)) = 1$ and $\rho(s)^\dagger = \rho(s)$, the number $\text{Tr}(\dot{U} U^\dagger)$ is purely imaginary. Hence, a necessary condition for parallel transport is

$$\text{Tr}(\dot{U}(s) U^\dagger(s) \rho(s)) = 0 \quad (5.4)$$

However, such a condition is not sufficient to fix $U(s)$ for a given $\rho(s)$. Indeed, considering any $N \times N$ matrix representation of the given ρ , Eq.(5.4) determines the $N \times N$ matrix U only up to N phase factors. In order to fix these factor we must impose a more stringent condition:

$$\langle k(s)|\dot{U}(s) U^\dagger(s)|k(s)\rangle = 0, \quad k = 1, \dots, N, \quad (5.5)$$

where $\rho(s) = \sum_k w_k |k(s)\rangle\langle k(s)|$. This gives the desired generalization of parallel transport to the case of mixed states. Eq.(5.4) reduces to $\langle \psi(s)|\dot{\psi}(s)\rangle = 0$ for a pure state $\rho(s) = |\psi(s)\rangle\langle \psi(s)|$. Indeed, Eq.(5.4) gives $\text{Tr}(\dot{U}(s) U^\dagger(s) \rho(s)) = \text{Tr}(U^\dagger(s) \dot{U}(s) \rho(0)) = 0$, so that for $\rho(0) = |\psi(0)\rangle\langle \psi(0)|$ we have $\text{Tr}(U^\dagger(s) \dot{U}(s) |\psi(0)\rangle\langle \psi(0)|) = \langle \psi(0)|U^\dagger(s) \dot{U}(s)|\psi(0)\rangle = \langle \psi(s)|\dot{\psi}(s)\rangle = 0$.

We can now define a geometric phase for a state tracing out the curve defined by the map $C : s \rightarrow \rho(s) = U(s) \rho_0 U^\dagger(s)$, with $s \in [s_1, s_2]$ and $U(s)$ satisfying Eqs.(5.4) and (5.5). The dynamical phase $\Phi_{dyn} \equiv -i \int_{s_1}^{s_2} ds \text{Tr}(U^\dagger(s) \dot{U}(s) \rho(0))$ then vanishes and we define the geometric phase Φ_g for mixed states as

$$\Phi_g = \arg \text{Tr}(U(s) \rho(0)). \quad (5.6)$$

Considering the ensemble decomposition $\rho(0) = \sum_k w_k |k(0)\rangle\langle k(0)|$ a look at Eq.(5.2) makes clear that we can write Φ_g in the form

$$\Phi_g = \arg \text{Tr}(U(s) \rho(0)) = \arg \left(\sum_k w_k v_k e^{i\gamma_k} \right), \quad (5.7)$$

with the geometric phase factors $e^{i\gamma_k}$ being associated with the individual pure-state paths followed by the members of the ensemble.

Φ_g is manifestly gauge and parametrization invariant and has been defined for open paths, in general. However it does not share all the properties of the geometric phase for pure states. In particular, it is not additive in the sense of Eq.(3.28). Nevertheless, in special cases it can be connected with a solid angle. Let us see an example of such a case.

Consider a two-level system. In this case

$$\rho = \frac{1}{2} (I + \vec{r} \cdot \vec{\sigma}) = \frac{1}{2} (I + r \vec{n} \cdot \vec{\sigma}), \quad (5.8)$$

with $\vec{n} \cdot \vec{n} = 1$ and r being constant for a unitary evolution U . For pure states $r = 1$, while $r < 1$ for mixed states. The unitary evolution of $\rho(s)$ makes $\vec{n}(s)$ to trace out a curve on the Bloch sphere. Suppose this curve is closed by joining its initial and final points with a geodesic, so that it subtends a solid angle Ω . Then, the two eigenstates $|\pm; \vec{n} \cdot \vec{\sigma}\rangle$ of $\vec{n} \cdot \vec{\sigma}$ acquire the geometric phases $\mp\Omega/2$, as we saw before. Both states have the same visibility $v_0 = |\langle \pm; \vec{n} \cdot \vec{\sigma} | U | \pm; \vec{n} \cdot \vec{\sigma} \rangle|$. From Eq.(5.7) we obtain, considering that in the present case the $w_{k=\pm}$ (the eigenvalues of ρ) are given by $w_{\pm} = (1 \pm r)/2$, the geometric phase

$$\Phi_g = \arg \left(\frac{1+r}{2} e^{-i\Omega/2} + \frac{1-r}{2} e^{+i\Omega/2} \right) = \arg \left[\cos \left(\frac{\Omega}{2} \right) - ir \sin \left(\frac{\Omega}{2} \right) \right] = -\arctan \left(r \tan \left(\frac{\Omega}{2} \right) \right). \quad (5.9)$$

and the visibility $v = |\text{Tr}(U\rho(0))|$, that is,

$$v = \left| \sum_{k=\pm} w_k v_k e^{i\gamma_k} \right| = v_0 \left| \frac{1+r}{2} e^{-i\Omega/2} + \frac{1-r}{2} e^{+i\Omega/2} \right| = v_0 \sqrt{\cos^2 \left(\frac{\Omega}{2} \right) + r^2 \sin^2 \left(\frac{\Omega}{2} \right)}. \quad (5.10)$$

Eqs.(5.9) and (5.10) reduce for $r = 1$ to $\Phi_g = -\Omega/2$ and $v = v_0$, respectively, the known expressions for pure states. For maximally mixed states, i.e., $r = 0$, we obtain $\Phi_g = \arg \cos(\Omega/2)$ and $v = |\cos(\Omega/2)|$, so that for the output intensity Eq.(5.3) gives

$$I = 2 + 2 |\cos(\Omega/2)| \cos(\phi - \arg \cos(\Omega/2)) = 2 + 2 \cos(\Omega/2) \cos \phi. \quad (5.11)$$

We see that for $\Omega = 2\pi$ there is a sign-change in the intensity pattern. This was experimentally observed in early experiments [16] testing the 4π symmetry of spin-1/2 particles.

Chapter 6

Off-diagonal geometric phases and geometric phase between orthogonal states

As we have seen, in the context Berry's original approach, a system undergoing adiabatic evolution under the action of a parameter-dependent Hamiltonian $H(s)$ accumulates a geometric phase. The instantaneous eigenstates of the Hamiltonian were denoted by $|n; R(s)\rangle$, that is, $H(R(s)) |n; R(s)\rangle = E_n(R(s)) |n; R(s)\rangle$, with R meaning the set of parameters and the eigenvalues E_n being assumed as non-degenerate. Let simplify this notation, by writing $H(s) |u_n(s)\rangle = E_n(s) |u_n(s)\rangle$. When $|u_n(s)\rangle$ is transported adiabatically along a closed loop $R(s_2) = R(s_1)$, the scalar product $\langle u_n(s_1) | u_n(s_2) \rangle$ acquires a nontrivial geometric phase factor. It is assumed that $\langle u_n(s_1) | u_n(s_2) \rangle \neq 0$; otherwise, the relative phase is not well defined. However, it might occur, for $n \neq m$, that $|u_n(s_2)\rangle = e^{i\alpha} |u_m(s_1)\rangle$. In such a case both $\langle u_n(s_1) | u_n(s_2) \rangle$ and $\langle u_m(s_1) | u_m(s_2) \rangle$ vanish, as $E_n(s_1)$ and $E_m(s_2)$ are non-degenerate, so that the Pancharatnam-Berry phase is undefined. If we are looking for phase information, then we should be able to extract it from the off-diagonal matrix element $\langle u_n(s_1) | u_m(s_2) \rangle$. This was done by Manini and Pistoiesi some years ago [7].

In the usual definition of the geometric phase one considers the parallel transport of a normalized state $|u_n(s)\rangle$ along a curve \mathcal{C} with $s \in [s_1, s_2]$. A state $|u_n^\parallel(s)\rangle$ that is parallel transported satisfies $\langle u_n^\parallel(s) | \dot{u}_n^\parallel(s) \rangle = 0$. It represents a particular lift of $|u_n(s)\rangle \langle u_n(s)|$, whose phase has been so chosen, that $\langle u_n^\parallel(s) | u_n^\parallel(s + \delta s) \rangle$ differs from unity up to terms of second order in δs . This means that the phase of $|u_n^\parallel(s + \delta s)\rangle$ is such that this state has maximal projection on the "previous" state $|u_n^\parallel(s)\rangle$. We can make this phase-choice explicit, by writing

$$|u_n^\parallel(s_2)\rangle = \exp \left[- \int_{s_1}^{s_2} \langle u_n(s) | \dot{u}_n(s) \rangle ds \right] |u_n(s_2)\rangle = \exp \left[- \int_{\mathcal{C}} \langle u_n(R) | \nabla |u_n(R)\rangle \cdot d\mathbf{R} \right] |u_n(s_2)\rangle. \quad (6.1)$$

The geometric phase is then given by $\arg \langle u_n^\parallel(s_1) | u_n^\parallel(s_2) \rangle$ or, equivalently, by the following phase factor that is defined in terms of the function $\Phi(z) = z/|z|$, for complex $z \neq 0$:

$$\gamma_n^C \equiv \Phi(U_{nn}^C) = \Phi \left(\langle u_n^\parallel(s_1) | u_n^\parallel(s_2) \rangle \right). \quad (6.2)$$

As we have seen, γ_n^C is gauge and parametrization invariant and is thus a measurable quantity.

The natural extension of γ_n^C appears to be the quantity $\sigma_{nm}^C \equiv \Phi(U_{nm}^C) = \Phi(\langle u_n^\parallel(s_1) | u_m^\parallel(s_2) \rangle)$; but such a quantity happens to be gauge dependent. Under gauge transformations $|u_n(s)\rangle \rightarrow \exp(i\alpha_n(s)) |u_n(s)\rangle$, it transforms as

$$\sigma_{nm}^C \rightarrow \sigma_{nm}^C \exp(i\alpha_m(s) - i\alpha_n(s)). \quad (6.3)$$

Manini and Pistolesi [7] defined thus a measurable quantity related to σ_{nm}^C , that is the proper generalization of γ_n^C , namely

$$\gamma_{nm}^C = \sigma_{nm}^C \sigma_{mn}^C, \quad (6.4)$$

and gave to it a simply geometric interpretation analogous to that of Pancharatnam's phase [7]. The simplest system on which off-diagonal phases could be tested is a spin-1/2 acted upon by a slowly rotating magnetic field whose orientation is so chosen that $\gamma_{n=1,2}^C$ are undefined and all the phase information is thus contained in γ_{12}^C . The theoretical predictions for this case have been experimentally confirmed [22].

The goal of circumventing the restriction of dealing with non-orthogonal states when defining geometric phases has been led a step further by Wong, Cheng and Chu [6]. These authors introduced a "projective phase" between two states $|\psi(0)\rangle$ and $|\psi(s)\rangle$, given by

$$\varphi_i(0, s) = \arg\langle\psi(0)|i\rangle\langle i|\psi(s)\rangle, \quad (6.5)$$

with $|i\rangle$ being some state to which neither $|\psi(0)\rangle$ nor $|\psi(s)\rangle$ are orthogonal, though they may be orthogonal to each other. The physical idea behind the definition of the projective phase is similar to the idea behind Pancharatnam's phase. In the latter case two states are taken to interfere with one another and then the amplitude $\langle\psi(s)|\psi(0)\rangle$ contains the phase difference. This goes as long as such an amplitude does not vanish. If it does, we can first project each of the states along a state $|i\rangle$, which is non-orthogonal to them, and take their projections, $|i\rangle\langle i|\psi(0)\rangle$ and $|i\rangle\langle i|\psi(s)\rangle$ to interfere. This leads to $\varphi_i(0, s)$.

Wong, Cheng and Chu proved [6] that the projective phases at two states, $|i\rangle$ and $|j\rangle$, are related to one another by the following gauge transformation:

$$\exp[i\varphi_i(0, s)] = S_{ij}(\psi(0)) \exp[i\varphi_j(0, s)] S_{ji}(\psi(s)), \quad (6.6)$$

with the transition functions being defined as

$$S_{ij}(\psi) = S_{ji}^{-1}(\psi) = \frac{\langle j|\psi\rangle\langle\psi|i\rangle}{|\langle j|\psi\rangle\langle\psi|i\rangle|} \quad (6.7)$$

The projective phase can be used to prove that the Pancharatnam phase-change that arises when passing through an orthogonal state is either π or zero (modulo 2π). Furthermore, all off-diagonal phases can be obtained from the projective phase. For details, we refer to the literature [6].

Chapter 7

Thomas rotation in relativity and in polarization optics

Let us address a well known effect of relativity and see how it can be understood in terms of notions related to geometric phases. We recall that Thomas rotation arose as a surprising effect that passed unnoticed for several years, even to Einstein himself [24]. It is a consequence of the structure of the Lorentz group of transformations. These transformations relate to each other two inertial reference systems, O and O' , whose respective coordinates we denote by x^μ and x'^μ with μ , as all Greek indexes in this Section, running from 0 to 3; $x^0 = ct$, and the x^i denoting spatial coordinates (Latin indexes run from 1 to 3). Both reference systems, O and O' , are related by a Lorentz transformation, which is defined as one that leaves the quadratic form $(x^0)^2 - (x^1)^2 - (x^2)^2 - (x^3)^2$ invariant. Let us write this form with the help of the metric tensor $\eta_{\mu\nu} = \text{diag}(1, -1, -1, -1)$ as $\eta_{\mu\nu}x^\mu x^\nu$, where we have used the convention that a sum is assumed over repeated indexes. A Lorentz transformation, $x^\mu \rightarrow x'^\mu = \Lambda^\mu_\nu x^\nu$ is given by those matrices Λ whose entries satisfy

$$\Lambda^\mu_\nu \eta_{\mu\tau} \Lambda^\tau_\sigma = \eta_{\nu\sigma}. \quad (7.1)$$

Lorentz transformations form a six-parameter Lie group, whose elements can be written as $\Lambda = \exp L$, with

$$L = -\vec{\omega} \cdot \vec{S} - \vec{\zeta} \cdot \vec{K}. \quad (7.2)$$

Here, \vec{S} and \vec{K} are the group generators, while $\vec{\omega} = (\omega_1, \omega_2, \omega_3)$ and $\vec{\zeta} = (\zeta_1, \zeta_2, \zeta_3)$ denote the six parameters in terms of which each group element is defined. The generators form an algebra, the Lie algebra of the group, which in the present case is defined through the following commutators:

$$[S_i, S_j] = \epsilon_{ijk} S_k, \quad (7.3)$$

$$[S_i, K_j] = \epsilon_{ijk} K_k, \quad (7.4)$$

$$[K_i, K_j] = -\epsilon_{ijk} S_k \quad (7.5)$$

In Eq.(7.3) we recognize the commutators of the $su(2)$ algebra, which is the algebra of the rotation group. Rotations are thus particular Lorentz transformations. On the other hand, the

K_i are generators of so-called “boosts”, those transformations which relate coordinate systems moving uniformly with respect to each other, and with their coordinate axes being parallel, i.e., $\vec{e}_x \parallel \vec{e}_{x'}$, etc. Intuitively, if O and O' are related by a boost, and so also O' and O'' , then we expect that the same holds true for the transformation relating O and O'' . That is, if $\vec{e}_x \parallel \vec{e}_{x'}$ and $\vec{e}_{x'} \parallel \vec{e}_{x''}$, then we expect that $\vec{e}_x \parallel \vec{e}_{x''}$. The surprising discovery of Thomas was that it is not the case. Being parallel is not a transitive property, in the frame of Lorentz transformations. Technically speaking, the product of two boosts is not a boost, but some Lorentz transformation that can be expressed as a product of a boost by a rotation, the Thomas rotation.

As almost all relativistic effects, in order to exhibit Thomas rotation we should consider two systems whose relative velocity is near the velocity of light: c . Otherwise, the effect is too small to be observed. However, there is an equivalent effect that appears in the context of geometric phases whose observation might be realizable with standard equipment. The root of Thomas rotation is the non-transitive property of boosts. As we have seen, Pancharatnam’s connection relates also in a non-transitive way two polarization states. Intensity-preserving transformations of these states form a representation of the rotation group $SU(2)$. But these are only particular transformations among more general ones which include intensity non-preserving transformations. The latter can be realized with the help of, e.g., polarizers, that is, *dichroich* optical elements. As we shall see, these elements provide us with the necessary tools for studying Thomas rotations in an optical framework.

Before we discuss the optical framework, we need some more algebra to build the bridge connecting Lorentz transformations with polarization transformations. To this end, we recall a Lorentz invariant, quantum mechanical equation, the Dirac equation:

$$(i\gamma^\mu \partial_\mu - m)\psi(x) = 0, \quad (7.6)$$

with $\psi(x)$ denoting a bi-spinor – a complex-valued four-component function of space-time x^μ – and the γ^μ being the Dirac matrices whose defining algebra is

$$\gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu = 2\eta^{\mu\nu}. \quad (7.7)$$

The vector space to which the bi-spinors $\psi(x)$ belong provides a representation-space for Lorentz transformations, just as space-time with vectors x^μ does. Whereas in the latter Lorentz transformations are represented by matrices $\Lambda = \exp L$, in bi-spinor space they are represented by matrices of the form

$$S(\Omega_{\mu\nu}) = \exp\left(-\frac{1}{4}\Omega_{\mu\nu}\gamma^\mu\gamma^\nu\right), \quad (7.8)$$

with the antisymmetric coefficients $\Omega_{\mu\nu}(\Lambda) = -\Omega_{\nu\mu}(\Lambda)$ representing the six independent parameters that define each element of the group, just as the parameters in $\Lambda = \Lambda(\vec{\omega}, \vec{\zeta})$ do.

The commutation properties of the γ^μ matrices allow us to write $S(\Omega_{\mu\nu})$ in terms of Pauli matrices $\vec{\sigma}$. This is so because $S(\Omega_{\mu\nu})$ contains only even products of the γ^μ matrices. Such products conform a subalgebra of the (Clifford) algebra formed by the γ^μ . This subalgebra is isomorphic to the Pauli-algebra (sometimes employed in polarization optics as *quaternion* algebra). We can then map each 4×4 matrix $S(\Omega_{\mu\nu})$ into a 2×2 matrix $T(\vec{\alpha}, \vec{\beta})$ given by

$$T(\vec{\alpha}, \vec{\beta}) = \exp\left[\left(\vec{\alpha} + i\vec{\beta}\right) \cdot \vec{\sigma}\right] \quad (7.9)$$

We see that $T(\vec{\alpha}, \vec{\beta})$ is like an element of $SU(2)$, $\exp\left[i\vec{\delta} \cdot \vec{\sigma}\right]$, but having three complex coefficients $(\vec{\alpha} + i\vec{\beta})$ in place of the three real ones $\vec{\delta}$. The complex coefficients $(\vec{\alpha} + i\vec{\beta})$

entail the six real parameters of the Lorentz group. The representation of this group by matrices of the form given in Eq.(7.9) is what we need to make the connection with polarization optics, where matrices of such a kind represent polarization transformations.

Polarization states corresponding to a monochromatic plane wave of light can be represented by two-component vectors with complex components: $(v_x \exp(i\phi_x), v_y \exp(i\phi_y))^T$, so-called *Jones vectors*. Physically, only the relative amplitude v_x/v_y and the relative phase $\phi_y - \phi_x$ matter, so that a polarization state can be given in the form:

$$|\pi\rangle = \begin{pmatrix} \cos \chi \\ e^{i\phi} \sin \chi \end{pmatrix}. \quad (7.10)$$

Alternatively, polarization states can be represented by four-component *Stokes vectors* (s_0, \vec{s}) , corresponding to a quantum-mechanical representation of pure states by density operators:

$$\rho = |\pi\rangle \langle \pi| = \frac{1}{2} (I + \vec{s} \cdot \vec{\sigma}). \quad (7.11)$$

Here, as we have taken a normalized ket $|\pi\rangle$ to represent the polarization state, $s_0 = \text{Tr}(|\pi\rangle \langle \pi|) = 1$. This is the coefficient of the identity matrix I in Eq. (7.11). In general, the Stokes four-vector $(s_0, \vec{s}) = (\text{Tr} \rho, \text{Tr}(\rho \cdot \sigma_1), \text{Tr}(\rho \cdot \sigma_2), \text{Tr}(\rho \cdot \sigma_3))$. For a $|\pi\rangle$ given as in Eq.(7.10), $\vec{s} = (\cos(\phi) \sin(2\chi), \sin(\phi) \sin(2\chi), \cos(2\chi))$. The set of unit vectors \vec{s} span the Poincaré-Bloch sphere and constitute a representation of polarization states (the standard Poincaré sphere in optics corresponds to choosing a representation of Pauli matrices $\vec{\rho}$ given by $\rho_1 = \sigma_3, \rho_2 = \sigma_1, \rho_3 = \sigma_2$).

Intensity preserving transformations, like those realized by wave plates – examples of these are quarter-wave plates (QWP) and half-wave plates (HWP) – are represented by 2×2 matrices belonging to the $SU(2)$ group. The effect of such a matrix on \vec{s} is to rotate it without changing its length. A general matrix of the group $SU(2)$ is given by $\exp(i\delta \vec{n} \cdot \vec{\rho}/2)$. Matrices $Q(\delta)$ and $H(\delta)$ representing a QWP and a HWP, respectively, are given by

$$Q(\delta) = \frac{1}{\sqrt{2}} [I - i \sin(2\delta) \sigma_1 - i \cos(2\delta) \sigma_3] \quad (7.12)$$

$$H(\delta) = -i \sin(2\delta) \sigma_1 - i \cos(2\delta) \sigma_3. \quad (7.13)$$

By applying $U = \exp(i\Phi \vec{n} \cdot \vec{\sigma}/2) = \cos(\Phi/2) I + i \sin(\Phi/2) \vec{n} \cdot \vec{\sigma}$ to an initial polarization vector $|\pi_i\rangle$ we obtain a transformed output vector $|\pi_o\rangle = U |\pi_i\rangle$. The corresponding Stokes vectors, \vec{s}_i and \vec{s}_o respectively, are related by the well-known Rodrigues formula [25] that gives a rotated vector in terms of the rotation angle and axis:

$$\vec{s}_o = \cos(\Phi) \vec{s}_i + [1 - \cos(\Phi)] (\vec{n} \cdot \vec{s}_i) \vec{n} + \sin(\Phi) \vec{s}_i \times \vec{n}. \quad (7.14)$$

This equation can be derived from

$$\begin{aligned} |\pi_o\rangle \langle \pi_o| &= \frac{1}{2} (I + \vec{s}_o \cdot \vec{\sigma}) = U |\pi_i\rangle \langle \pi_i| U^\dagger \\ &= \left(\cos\left(\frac{\Phi}{2}\right) I + i \sin\left(\frac{\Phi}{2}\right) \vec{n} \cdot \vec{\sigma} \right) \frac{1}{2} (I + \vec{s}_i \cdot \vec{\sigma}) \left(\cos\left(\frac{\Phi}{2}\right) I - i \sin\left(\frac{\Phi}{2}\right) \vec{n} \cdot \vec{\sigma} \right) \end{aligned} \quad (7.15)$$

Consider now dichroic optical elements like a non-ideal polarizer. To encompass optical conventions [26] let us use in what follows the $\vec{\rho}$ Pauli matrices: $\rho_1 = \sigma_3, \rho_2 = \sigma_1, \rho_3 = \sigma_2$. In such a representation the polarization vector as given in Eq.(7.10) corresponds to being x -polarized

when $\chi = 0$ and y -polarized when $\chi = \pi/2$. In this case the matrix representing a non-ideal polarizer whose lines of maximal and minimal transmission coincide with the x - and y -polarization axes, respectively, is given by

$$J_{diag} = \begin{pmatrix} p_x & 0 \\ 0 & p_y \end{pmatrix}. \quad (7.16)$$

The eigenvectors of J_{diag} , $(1, 0)^T$ and $(0, 1)^T$, are thus polarization vectors along the x and $-x$ directions, respectively, on the Poincaré sphere. In order to obtain the corresponding matrix whose eigenvectors are $|\pi_1\rangle = (\cos \chi, e^{i\phi} \sin \chi)^T$ and its orthogonal vector $|\pi_2\rangle = (-e^{-i\phi} \sin \chi, \cos \chi)^T$, we submit J_{diag} to the unitary transformation

$$J = U J_{diag} U^\dagger, \quad (7.17)$$

with U being the matrix whose columns are $|\pi_1\rangle$ and $|\pi_2\rangle$:

$$U = \begin{pmatrix} \cos \chi & -e^{-i\phi} \sin \chi \\ e^{i\phi} \sin \chi & \cos \chi \end{pmatrix}. \quad (7.18)$$

This gives for J a matrix that can be written as

$$J = \left(\frac{p_x + p_y}{2} \right) I + \left(\frac{p_x - p_y}{2} \right) [(\cos 2\chi) \rho_1 + (\sin 2\chi \cos \phi) \rho_2 + (\sin 2\chi \sin \phi) \rho_3]. \quad (7.19)$$

Assuming that the transmission axis is x , i.e., that $p_x > p_y$, we write $p_x = \exp(-\alpha_<)$, $p_y = \exp(-\alpha_>)$ and set $\vec{\Gamma} = (\cos 2\chi, \sin 2\chi \cos \phi, \sin 2\chi \sin \phi)$. Then,

$$J = \exp\left(-\frac{\alpha_> + \alpha_<}{2}\right) \left\{ \cosh\left(\frac{\alpha_> - \alpha_<}{2}\right) I + \sinh\left(\frac{\alpha_> - \alpha_<}{2}\right) \vec{\Gamma} \cdot \vec{\rho} \right\}. \quad (7.20)$$

Now, Eq.(7.9) can be shown to be just of this form. Indeed, in order to show this we write $T(\vec{\alpha}, \vec{\beta}) = \exp(-\vec{f} \cdot \vec{\rho})$, with $\vec{f} = \vec{\alpha} + i\vec{\beta}$. The matrix $\vec{f} \cdot \vec{\rho}$ has the following (in general complex) eigenvalues:

$$\lambda_{\pm} = \pm \sqrt{(\vec{\alpha}^2 - \vec{\beta}^2 + 2i\vec{\alpha} \cdot \vec{\beta})} \equiv \pm z. \quad (7.21)$$

Let us denote by $|\mathbf{f}_{\pm}\rangle$ the eigenvectors of $\vec{f} \cdot \vec{\rho}$; that is, $(\vec{f} \cdot \vec{\rho}) |\mathbf{f}_{\pm}\rangle = \lambda_{\pm} |\mathbf{f}_{\pm}\rangle$. Thus, we have

$$I = |\mathbf{f}_+\rangle \langle \mathbf{f}_+| + |\mathbf{f}_-\rangle \langle \mathbf{f}_-| \quad (7.22)$$

$$\vec{f} \cdot \vec{\rho} = \lambda_+ |\mathbf{f}_+\rangle \langle \mathbf{f}_+| + \lambda_- |\mathbf{f}_-\rangle \langle \mathbf{f}_-|. \quad (7.23)$$

Solving for $|\mathbf{f}_{\pm}\rangle \langle \mathbf{f}_{\pm}|$ it follows that

$$|\mathbf{f}_{\pm}\rangle \langle \mathbf{f}_{\pm}| = \frac{zI \pm \vec{f} \cdot \vec{\rho}}{2z} \quad (7.24)$$

We apply now the general decomposition $\exp A = \sum_n \exp a_n |a_n\rangle \langle a_n|$ to the present case, i.e., $A = -\vec{f} \cdot \vec{\rho}$. The operator $\exp(-\vec{f} \cdot \vec{\rho})$ has eigenvectors $|\mathbf{f}_{\pm}\rangle$ and eigenvalues $\exp(\mp z)$. Thus,

$$\begin{aligned}
\exp(-\vec{f} \cdot \vec{\rho}) &= e^{-z} |\mathbf{f}_+\rangle \langle \mathbf{f}_+| + e^z |\mathbf{f}_-\rangle \langle \mathbf{f}_-| = \frac{e^{-z}}{2z} (zI + \mathbf{f} \cdot \vec{\rho}) + \frac{e^z}{2z} (zI - \vec{f} \cdot \vec{\rho}) \\
&= \left(\frac{e^z + e^{-z}}{2} \right) I - \left(\frac{e^z - e^{-z}}{2z} \right) \vec{f} \cdot \vec{\rho} = \cosh z - \sinh z \left(\frac{\vec{f}}{z} \right) \cdot \vec{\rho} \quad (7.25)
\end{aligned}$$

The Lorentz transformation that $\exp(-\vec{f} \cdot \vec{\rho})$ represents can generally be written as a product of a boost by a rotation. It is clear from Eq.(7.9) that a rotation is obtained when $\vec{\alpha} = \vec{0}$ and a boost when $\vec{\beta} = \vec{0}$. As we have seen, a general rotation $U \in SU(2)$ can be implemented with the help of three wave-plates as $Q(\beta_3)H(\beta_2)Q(\beta_1)$, see Eq.(4.6). A general boost can be implemented with dichroic elements that realize the transformation given in Eq.(7.20). The global factor there, $\exp(-(\alpha_> + \alpha_<)/2)$, corresponds to an overall diminution of intensity only. We can thus realize any $\exp(-\vec{f} \cdot \vec{\rho})$ by using optical elements like wave-plates and dichroic elements. In particular, by letting a polarization state pass through two consecutive dichroic elements – each corresponding to a boost – we could make appear a phase between initial and final polarization states. This is a geometric phase whose origin is a rotation induced between the polarization states: a Thomas rotation. Such an effect can thus be easily exhibited in the domain of polarization optics, in contrast with the relativistic case, where one needs to reach velocities near the velocity of light. Moreover, we have here another nice example showing the common topological root of two phenomena, that at first sight might appear to be unrelated to one another.

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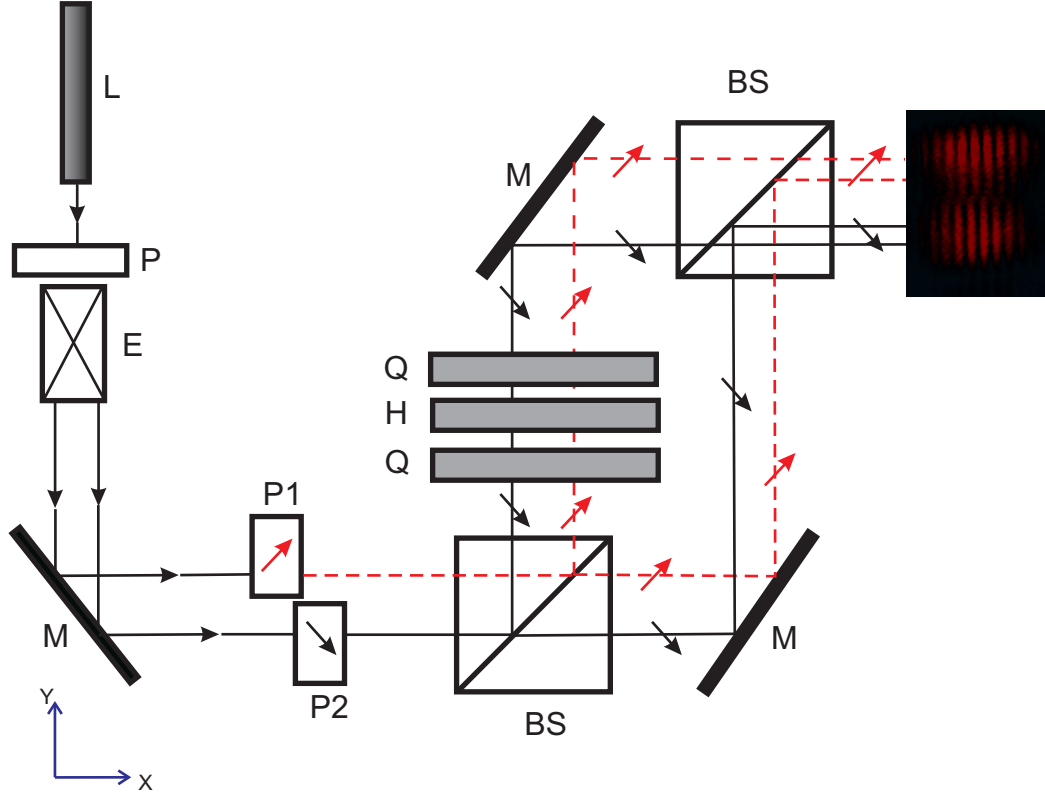


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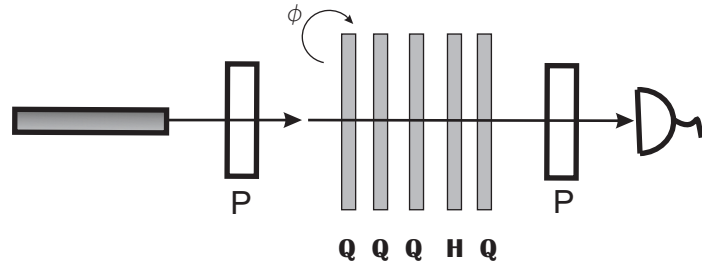


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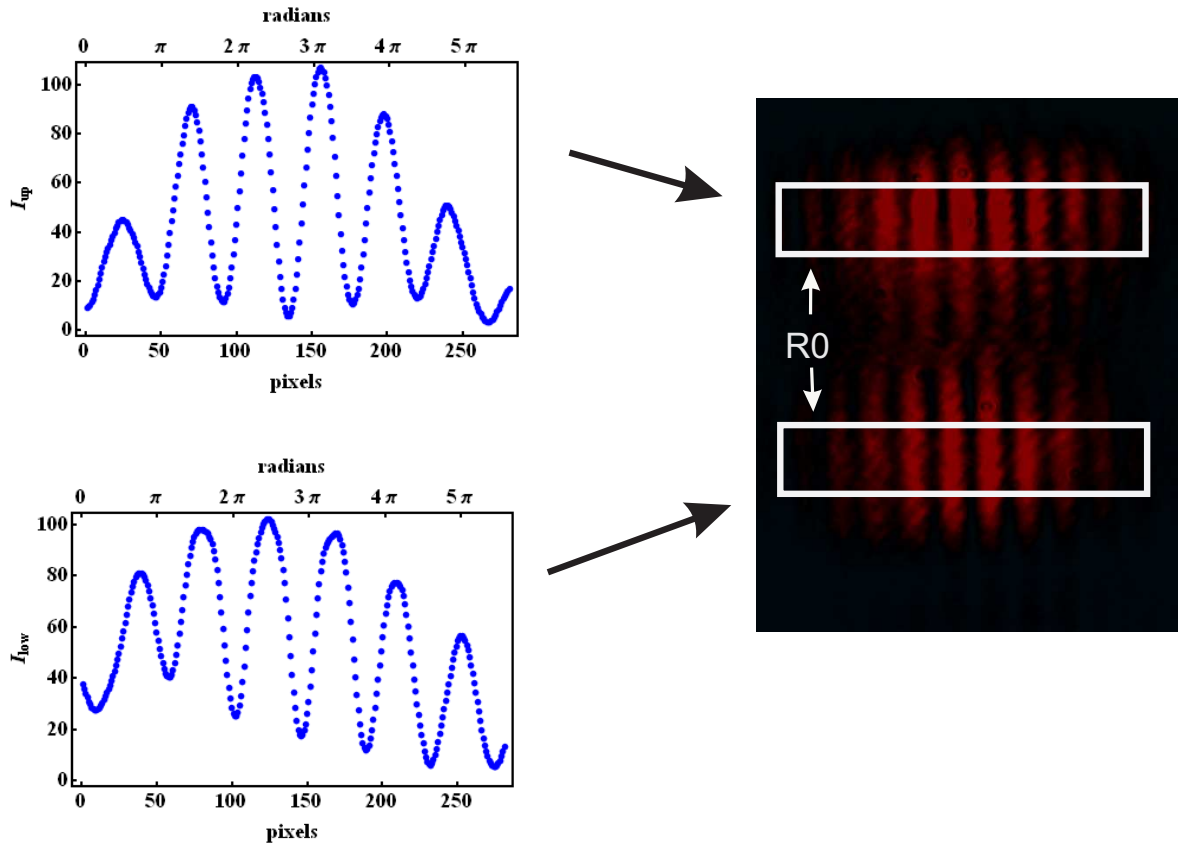


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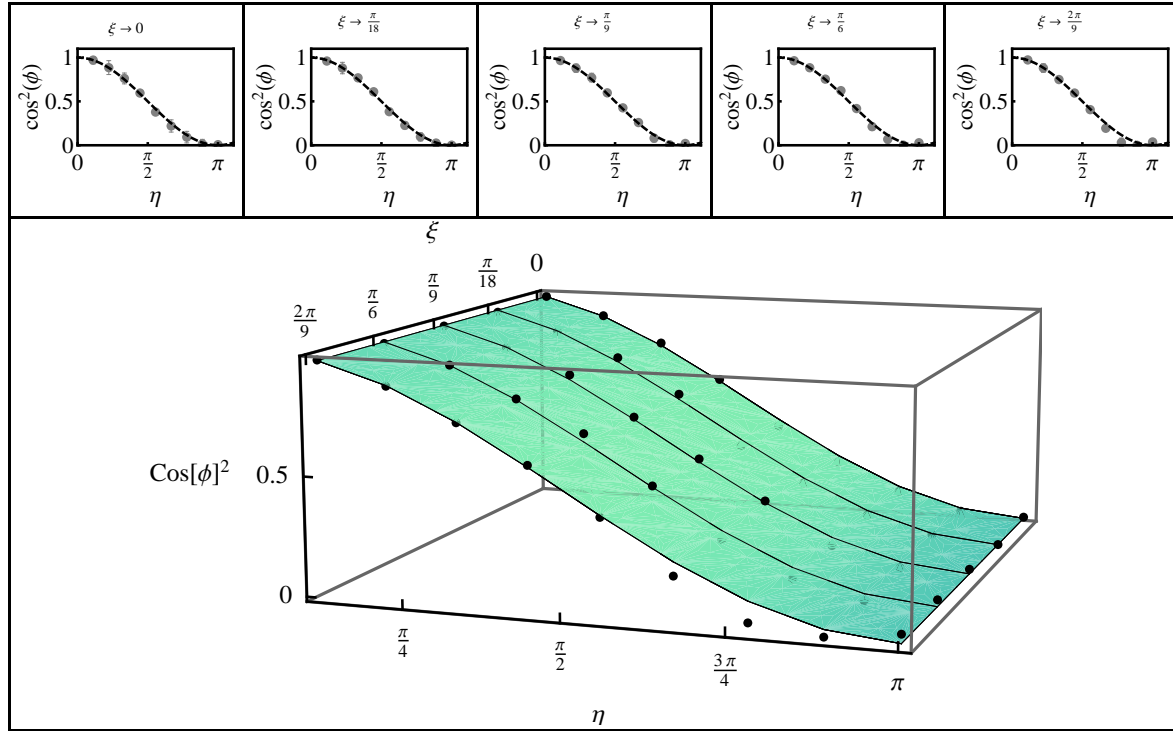


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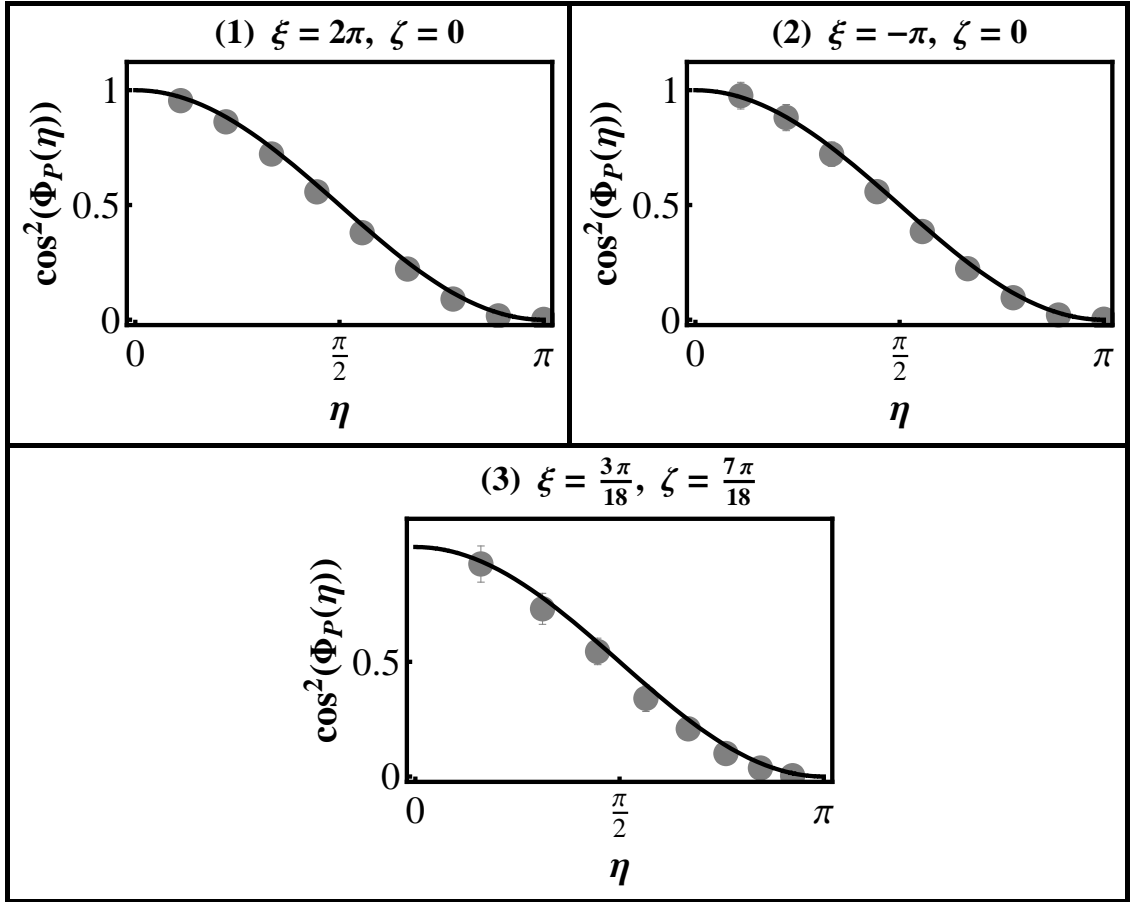


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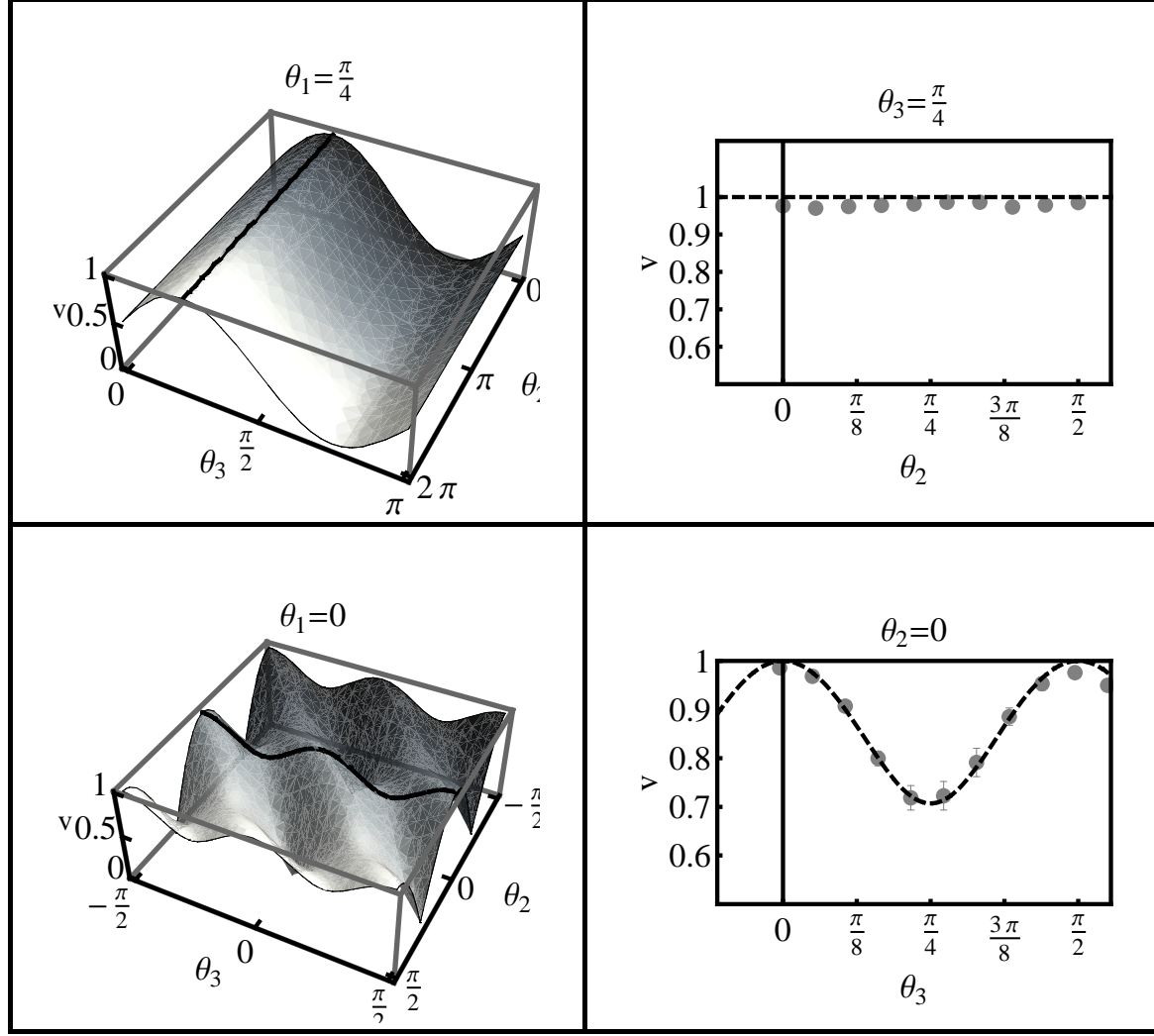


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